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The Publication of the International
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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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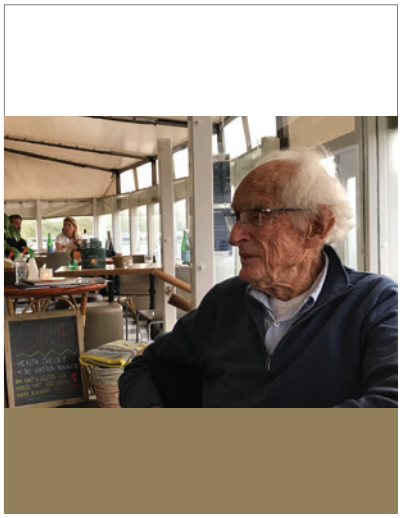

On May 2, 2020, Professor Joan van der Waals, Fellow of the International EPR(ESR) Society and Zavoisky Awardee 1999, celebrated his 100th birthday. Happy birthday to you, Professor van der Waals!

Photo courtesy of Silvia Völker.

epr newsletter

The Publication of the International EPR (ESR) Society

volume 30 number 3 2020

Editorial

Dear colleagues,

Joan van der Waals celebrated his 100th birthday on May 2nd, 2020. It is understandable that this fantastic anniversary of a patriarch of magnetic resonance, IES Fellow of 1996 (8/2, p. 4), is of top urgency in our publication. The cover picture clearly indicates that the Anniversaries column is the highlight of this issue. Edgar Groenen and Jan Schmidt describe the contributions of Joan van der Waals to EPR and underline his role in their scientific careers (pp. 5, 6). Joan's interview is a special treat to our readership, particularly the younger generation of magnetic resonance researchers (p. 7). Thomas Prisner and Keith McLauchlan join Edgar and Jan with heartfelt congratulations and details of their personal contacts with Joan (p. 8). More colors to Joan's portrait are added by the article of Mel Voet on the occasion of Joan's 99th birthday we reproduce from MARE, journal of the Leiden University (pp. 9, 10).

Back to the cover picture: I like this photo of Joan. There is a saying that there are two things you can watch for eternity: fire and water. I would add the third thing: a face of a man, who was born one hundred years ago, in deep thought. It is History alive. I am fascinated by the story of Joan's life. In the same way as I was fascinated in 1999 trying to contact Joan to inform him that he was chosen as the Zavoisky Awardee 1999 and getting the response that it was not possible to immediately relay this information to him because he was sailing on the high seas at the time. Sailing is his other passion, and you will certainly enjoy his article "Venturing by Sailboat into the Heart of Russia" (13/4, pp. 6, 7). Yes, our greats teach us valuable lessons of being ever young and interested in life and in science. Happy birthday to you, dear Joan! Take care, keep safe and stay healthy!

By now you must have received your copies of the *EPR newsletter* 30/1-2. I presume it was a pleasant surprise for you to find color in the body text. Yes, it is not a mirage. Now the newsletter is printed in full color. This metamorphosis is due to the activities of Aharon Blank, IES Secretary, on searching means to reduce mailing costs of the newsletter. As a result, he found not only an option to mail copies worldwide from Israel (mailing costs from Israel are lower than those from the States) but also an option to move printing from the States and print the newsletter in full color at the Printing Unit of Technion in Haifa.

We may say that 2020 opens a new era of the *EPR newsletter* production where we can offer full color in the newsletter to you, our dear readers. The previous transformation occurred in 2003, when we printed the *EPR newsletter* 13/1-2, the first issue of our publication with a color hard cover, at La Plume and Sons Printing in Lawrence, MA. The cover, originally printed in color only on the front and back, is paid for by Bruker. After some time producing the newsletter our long-term printers, LaPlume and Sons Printing was able to make a minor printing adjustment allowing for full color on the entire cover at no additional cost. Switching to a silk coated stock also improved the printability and look of the newsletter. For seventeen years we enjoyed collaboration with Scott Morton and his highly professional and efficient team. We printed seventeen volumes, from 13th to 29th, at LaPlume, and all paying members of the IES got high-quality copies of our newsletter. In this issue, we say a big thank-you to LaPlume, Scott Morton and his team. We terminate printing the newsletter at LaPlume but this does not terminate our deep feelings of mutual understanding and friendship.

Heartfelt thanks to you, Scott! We wish you and your team all the best!

Laila Mosina

John Weil Young Investigator Award 2020

Sabine Richert

I am honoured to have been selected by the International EPR (ESR) Society to receive the 2020 John Weil Young Investigator Award for my doctoral and postdoctoral work in the field of EPR spectroscopy. While I am very grateful for this recognition, I am also aware that most of this work could not have been accomplished without the help and guidance of the people who surrounded me during the past years. I would therefore like to use this contribution not only to present a scientific overview of my research but also to thank my colleagues and friends in the EPR community for their continued support.

My scientific journey started at the Graz University of Technology in Austria where I completed my Masters' thesis in 2010, in the area of photochemistry and spin chemistry, looking at time-dependent magnetic field effects on the exciplex fluorescence in organic donor-acceptor pairs [1]. I then moved to Geneva to work as a research assistant on the study of ultrafast photochemical processes in liquid solution and at liquid/liquid interfaces, before starting my doctorate in 2013 in the group of Professor Christiane Timmel at the University of Oxford. During my doctorate, I was introduced to pulse EPR spectroscopy and was fortunate to be given the possibility to work on a number of different research projects which also allowed me to put my photochemical background knowledge to good use.

Using various continuous-wave and pulse EPR techniques, I explored the molecular geometry, metal-ligand interactions, electronic communication and quantum interference phenomena in a range of linear and cyclic copper-containing multi-porphyrin arrays [2–5]. From the study on a ten-membered porphyrin nanoring with two copper and eight zinc centres, we learned that copper porphyrins can be suitable spin labels and that the Cu-Cu distance can be controlled precisely by the addition of different molecular templates. This control over the structure of the rigid supramolecular complexes, formed between the nanoring and the templates, is governed by differences in metal-ligand binding strength between zinc and copper to the axial nitrogen ligands of the template [2].

Since the previous study suggested that such rigid, cyclic porphyrin structures are ideal model compounds for the study of long-range electronic communication, we set out to explore the magnetic interactions in a six-membered porphyrin nanoring with two copper centres in opposing positions. Using DEER, we were indeed able to observe long-range electronic communication over a through-bond distance of 3.9 nm. Through simulations of the dipolar traces, in collaboration with Professor Ilya Kuprov at the University of Southampton, the exchange and dipolar interactions in this system could be quantified. The comparison of the magnitude of J with that obtained for an almost identical structure with only one coupling path between the copper centres, allowed us to conclude that the interaction in this cyclic system with two identical, parallel coupling paths is the result of constructive quantum interference [4].

In collaboration with the group of Professor Gunnar Jeschke at ETHZ, we were further able to show that ELDOR-detected hole burning can be used to quantify dipolar and exchange interactions in rigid porphyrin dimer systems [5].

In the second part of my doctorate, I combined photoexcitation and pulse EPR to study the factors influencing the extent of triplet state delocalisation in different types of linear porphyrin oligomers designed to act as molecular wires [6–9]. Making use of the complementary information provided by the zero-field splitting and the hyperfine interactions, we could show, on the example of porphyrin dimers with different end groups, that the triplet spin density will be unevenly distributed as soon as a slight electronic asymmetry is introduced in the system [8]. This implies that even delocalisation of the triplet state is limited to about two units in linear singly-bridged porphyrin oligomers.

In an additional study, we investigated fully conjugated zinc porphyrin tapes and their singly-bridged synthetic precursors [9]. We found that it is possible to force localisation of the triplet state on a single unit if the dihedral angle between adjacent porphyrin units gets close to 90 degrees. On the other hand, even delocalisation of the triplet wavefunction over more than two porphyrin macrocycles seems to require the formation of additional covalent bonds to reach electronic conjugation, as it is the case in the linear porphyrin tapes.

My interest in combining photoexcitation and EPR evolved even further during my postdoctoral time, both at the Universities of Oxford and Freiburg, where I was involved in a number of collaborative projects making use of different applications of transient EPR [10–12].

In December 2019, I started my independent career at the University of Freiburg as a junior research group leader with a fellowship from the German research foundation (DFG). My current research combines optical spectroscopy and pulse EPR with the aim to study the molecular requirements for spin-information transfer in photogenerated multi-spin systems.

Photogenerated multi-spin systems hold great promise for a range of technological applications in various fields, including molecular spintronics and artificial photosynthesis. In order to develop these applications further, we need to achieve photocontrol over the molecular magnetic properties of the materials to be used. However, this will only be possible if we manage to understand how and to which extent the molecular properties of the individual building blocks affect the underlying photophysics and excited state reaction mechanisms.

Profiting from the time-resolution of femtosecond transient UV-vis absorption and the capability of EPR to distinguish near-degenerate states with different spin multiplicity and characterise their spin-spin interactions, we are able to capture the internal dynamics of the studied systems from the femtosecond to the microsecond timescale, which provides us with a complete set of mechanistic information [13].

Our long-term goal is to establish design protocols for new magnetic materials, relating the molecular structure of the chemical system

to its ability to store and transfer quantum information efficiently.

I look forward to sharing our most recent results on this topic at one of the EPR conferences in the near future and would like to finish by thanking all my mentors and collaborators who contributed directly or indirectly to my scientific destiny. A special thanks goes to my thesis supervisor, Professor Christiane Timmel, for being extremely supportive and motivating not only during the time of my doctorate but well beyond, and to Professor Stefan Weber for hosting me and my group in his laboratories and generously providing access to his EPR instrumentation and equipment.

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Christiane Timmel:

Sabine graduated from the Graz University of Technology with top first class honours before working as a research assistant in the group of Professor Vauthey in Geneva. Upon her arrival in Oxford's Centre for Advanced Electron Spin Resonance, Sabine proved herself very quickly to be an exceptionally talented student, equally at home in Electron Spin Resonance and optical spectroscopies, techniques she exploited to the full during her doctorate studies in my group. Sabine impressed all peers and collaborating academics with her sheer unparalleled determination and diligence combined with admirable self-motivation and concentration. Her doctorate research output (11 publications in just 34 months of doctorate work in my group) tell only part of the story. The quality of the results obtained led to publications in high profile journals throughout, including Nature Communications, JACS and Chemical Science. She left Oxford to work in Stefan Weber's group in Freiburg before being awarded an Emmy Noether Fellowship to start her own research group in Freiburg.

Sabine has now published a total of 28 papers, just 7 years after her starting in Oxford as a doctoral student. She has been able to achieve this not only through her excellent scientific, mathematical and experimental skills but she impresses through unique efficiency in all she does, never wasting any time, literally concentrating on only the tasks in front of her. As a result she finished her doctorate in record time, and in outstanding quality whilst also serving as a key figure in the organisation of the 50th anniversary conference of the RSC ESR group held in Oxford. I do not know what we would have done without her! I did never have to give second thought to the conference brochure – or any other paperwork for that matter. I knew it was in Sabine's capable hands. The result was splendid, professional, organised, flawless.

In summary, Sabine is an exceptional scientist – sharp, dedicated, talented, versatile, concentrated. As at home in ESR as in laser spectroscopy she is a physical science all-rounder who has now begun to grow into an established and successful academic. I was lucky to share some of her academic journey and for that I will always be grateful.

2019 Tilden Prize Winner

Professor Eric McInnes
The University of Manchester, UK

Awarded for seminal contributions to the electron paramagnetic spectroscopy of transition metal compounds

2020 Tilden Prize Winner

Professor Christiane Timmel
University of Oxford, UK

Awarded for seminal contributions to fields of spin chemistry and electron paramagnetic resonance

IES Best Paper Award 2019–2020

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Dr. Fei Kong
University of Science and Technology of China

for the paper "Kilohertz electron paramagnetic resonance spectroscopy of single nitrogen centers at zero magnetic field", Science Advances 27 May 2020 Vol. 6, no. 22, eaaz8244 (additional authors Pengju Zhao, PeiYu, Zhuoyang Qin, Zhehua Huang, Zhecheng Wang, Mengqi Wang, Fazhan Shi, and Jiangfeng Du)

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Dr. Jason W. Sidabras
MPI Mulheim,

for the paper "Extending electron paramagnetic resonance to nanoliter volume protein single crystals using a self-resonant microhelix", Science Advances 04 Oct 2019: Vol. 5, no. 10, eaay1394 (additional authors Jifu Duan, Martin Winkler, Thomas Happe, Rana Hussein, Athina Zouni, Dieter Suter, Alexander Schnegg, Wolfgang Lubitz, and Edward J. Reijerse)

The contributions of Joan van der Waals to EPR: on the Occasion of His 100th Birthday

On Saturday the 2nd of May Joan Henri van der Waals celebrated his 100th birthday. At the occasion of this remarkable event it seems appropriate to describe his most remarkable contributions to the field of EPR during his scientific life.

After the war Joan finished his studies at the University of Amsterdam and joined the "Koninklijke Shell Laboratorium Amsterdam (KSLA)". He obtained his doctoral degree at the University of Groningen in 1950 with a thesis titled "Thermodynamic properties of mixtures of alkanes differing in chain length". He then worked on the description of clathrates and hydrates resulting in 1959 in the Van der Waals-Platteeuw clathrate hydrate theory. This theory attracted considerable attention because clathrates promised to be an attractive means to store natural gases like methane.

Meanwhile Joan was appointed as director of the department of fundamental research of the KSLA. He quickly realized the importance of NMR and he played an active role in stimulating the introduction of NMR as a tool for the research. The first Varian 60 MHz NMR spectrometer in The Netherlands was installed in his laboratory.

He developed a keen interest in the ideas of Lewis and Kasha who had suggested that the phosphorescence of organic molecules originates in the presence of a photo-excited metastable triplet state. Together with Menno de Groot, a gifted experimentalist, and using one of the first Varian EPR spectrometers available at the KSLA, they started the search for EPR signals of this elusive triplet state. Since at the time it was not clear how to incorporate a phosphorescent molecule in a host crystal, they decided to dissolve naphthalene in a glassy solution. Joan realized the handicap of the randomly oriented naphthalene molecules and the resulting dispersion of the EPR signals. At the time only few people realized that the presence of the zero-field splitting causes a severe broadening of the EPR lines. The limited sensitivity of the EPR spectrometers in those days made it almost impossible to observe the EPR transitions.

The brilliant idea of Joan was to search for the "$\Delta m = 2$" transition in the triplet state that exhibits an almost negligible dispersion. This search was successful and in 1959 they detected the EPR signals of the triplet state of naphthalene dissolved in a glassy host. Unknown to them, Clyde Hutchison and Bill Magnum at the University of Chicago reported in 1958, only half a year earlier, the observation of the EPR signals of naphthalene dissolved in a single crystal of durene. The experiments in Chicago and Amsterdam confirmed beyond doubt the triplet character of the phosphorescent state. Since that time EPR spectroscopy became a standard technique to study photo-excited triplet states.

The optical detection of EPR transitions in excited states was first suggested by Brossel and Kastler in 1949. A few years later, in 1952, Brossel and Bitter observed the transitions between sublevels of the $^3P_1$ excited state in a gas of mercury atoms. In 1959 the same method was applied to solids by Geschwind, Collins and Schawlow who found EPR transitions in the E(^{2}E) excited state of Cr^{3+} ions in Al_2O_3.

Of course many people were aware of the optical detection experiments of Brossel and Kastler and Geschwind *et al.* and it was suggested that similar experiments might be feasible for the metastable triplet state of ▶

Joan van der Waals at the occasion of his birthday in front of his house in Leiden (photo Bruno Wayenburg).

aromatic molecules. In the book "The Triplet State" published by Cambridge University Press in 1967 one can find an article by Jen *et al*. in which negative results were reported of an attempt to detect EPR of phosphorescent triplet-state molecules. In the same book a remarkable paper can be found by Joan van der Waals in which he explains the role of spin-orbit coupling and symmetry that determine the emissive properties of the triplet sublevels. In particular he shows that the phosphorescent emission of the triplet state is linearly polarized in contrast to the emission of the $^3P_1$ state of mercury atoms that is circularly polarized.

In 1967, Sharnoff observed the "$\Delta m = 2$" transitions in the triplet state of naphthalene as a change of its phosphorescence. In the same year the "$\Delta m = 1$" transitions in phosphorescent phenanthrene were detected optically by Kwiram and in phosphorescent quinoxaline by Joan van der Waals and collaborators at the KSLA. The simplicity of the optical detection of magnetic resonance or ODMR technique stimulated research groups worldwide to start ODMR on photo-excited triplet-state molecules.

In 1967, Joan van der Waals was appointed professor in experimental physics at Leiden University. Here he started a research group to study the properties of molecules in excited states with optical and magnetic-resonance techniques. He was convinced that the apparent advantages of optical methods over wide-band microwave detection systems would be particularly suited for the observation of the transitions between the spin sublevels of photo-excited triplet states in zero-magnetic field. Since the zero-field splitting does not depend on the orientation of the molecule, it was also expected that in this way the zero-field transitions could be observed in a great variety of phosphorescent molecules for which a suitable host crystal was difficult to find.

In 1968, the first successful ODMR experiment in his laboratory on a phosphorescent triplet-state molecule in zero-magnetic field was published. This first attempt was made on quinoline in a host crystal of durene. Many other research groups were inspired by this result. In the next decade hundreds of publications appeared in which ODMR experiments in zero-magnetic field were reported. In particular, this ODMR technique turned out to be extremely useful to elucidate the mechanism responsible for the radiative and non-radiative properties of the magnetic sublevels of phosphorescent triplet states. These findings confirmed the theoretical ideas of Joan presented in his paper in the book "The Triplet State" in 1967.

The observation of zero-field transitions of triplet-state molecules in glassy hosts turned out to be more difficult than expected. Strain in these solutions affects the size of the dipole-dipole interaction responsible for the zero-field splitting. Joan found an elegant solution to minimize this effect by incorporating phosphorescent molecules in Shpol'skii matrices. These matrices consist of normal alkanes in which the guest molecule replaces one or two alkane molecules. This idea worked especially well for the observation of magnetic-resonance signals of the triplet state of porphyrin molecules and an impressive number of papers appeared on a whole series of free-base and metal porphyrins.

In 1962, Joan received the Bourke Award of the Faraday Society. In 1971, he was elected member of the section Natural and Technical Sciences of the Koninklijke Nederlandse Akademie van Wetenschappen (Royal Netherlands Academy of Sciences). In 1985, he was appointed Knight in the Order of the Netherlands Lion. In 1996, he was elected a Fellow of the International EPR(ESR) Society. Since 1998 he has been an honorary member of the Royal Netherlands Chemical Society. In 1999, he received the Zavoisky Award for his outstanding contributions to EPR.

When looking back at the achievements of Joan van der Waals in the field of EPR one can only be surprised by his many talents. He is gifted by a brilliant mind that has led to an amazing variety of ideas and insights. He has been a stimulating scientist for colleagues all over the world and an inspiring leader for his collaborators, not the least the two of us.

I, Edgar Groenen, first met Joan when I was a master student in theoretical chemistry at Leiden University and took part in his course "Group theory and the application to atoms, molecules and crystals". He initiated my interest in the far-reaching consequences of symmetry, the beauty of the full rotation group and the concept of angular momentum. Some 15 years later, after my appointment at the physics department of Leiden University, we studied the lowest triplet state of a single crystal of C_{60} by electron-spin-echo detected EPR at 95 GHz. It took me some time to come up with an interpretation of the data, and symmetry considerations were essential. After a critical discussion, Joan approved my idea that the triplet state is delocalized over two neighbouring C_{60} molecules. As this example shows, also after his retirement, Joan continues to be a stimulating person to speak to.

I, Jan Schmidt, first met Joan when I applied for a job after finishing my military service. To my great surprise he not only offered me a position in the department of fundamental research of KSLA, but he also promised to send me to the then famous group of Anatole Abragam in Paris. I was so lucky that Ionel Solomon, "the long-legged spinner" as Professor Abragam used to call him, accepted me. In his laboratory I learned the secrets of the NMR and EPR techniques. Back in Amsterdam I decided to follow Joan to Leiden University where he had just started his research group. He supervised the completion of my thesis. He has always been my friend and trusted advisor, also when I took over the responsibility for the group after his retirement.

Edgar Groenen and Jan Schmidt

Interview with Professor Joan van der Waals on the Occasion of His 100th Birthday

EPR newsletter: *Dear Professor van der Waals, on behalf of the readers of the EPR newsletter we congratulate you on your 100th birthday. We are most appreciative that you agreed to answer the questions of this interview.*

Thank you very much for your congratulations with my 100-th birthday! Because of the Corona lock-down I was bound to the house (luckily with a garden) with only a few official visitors at the front door.

First of all I am not a typical magnetic resonance specialist. The transistor was discovered after I finished my university studies and my knowledge of electronics at the time I did my research was outdated. In the laboratory I was for technical matters greatly helped by others.

Now let me turn to your questions and give brief impromptu answers.

Why did you start towards your career in science?

At a young age I was already doing (sometimes dangerous!) experiments with electricity and building simple radios. At the age of about 12–14 my father and I used to read books together in the evening, once a week. I was captured by the popular book *De Bouw der Atomen* (*The Structure of the Atoms*) by Kramers and Helge Holst. This was exactly what I wanted in science: an accurate mathematical description of the phenomena!

Who introduced you into magnetic resonance?

After the war I joined Shell, which had their main research establishment (KSLA) in Amsterdam. In the winter of 1953/1954 I was enjoying an exchange year at Shell Development's laboratory in Emeryville, California. In the lab' I shared a room with Harden McConnell when in that room the first commercial NMR machine was installed, the Varian #1! We made up a tiny group of physicists who studied the the theoretical aspects and 'Mac' and I had many private discussions related to NMR and quantum physics. Needless to say that this sold magnetic resonance to me!

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

Here I have to disappoint the readers of the EPR newsletter. Looking back more than half a century, it is unquestionable that my theory of the stability of clathrates, and of the so-called gas-hydrates in particular, is pre-eminent amongst all I did. Clathrates are *solutions*, and their equilibrium composition for a given gas mixture can be calculated with a theoretical model based on the Lennard-Jones and Devonshire Quasi-crystalline theory for liquids (for details see: J. H. van der Waals and J. C. Platteeuw, Adv. Chem. Phys. **2** (1959), 1–57).

At the time we did it, our work on the triplet state got considerable attention. First with Menno de Groot by conventional EPR in an external magnetic field. Then the realization that the external field was an unnecessary evil when studying the spin sub-levels and the ensuing variable-frequency experiments with Jan Schmidt in Leiden.

When looking back we see a continuing interest in our work on clathrates; the theoretical part of the review article with Joost Platteeuw is almost cited verbatim in E. D. Sloan's text book on Gas Hydrates. What apparently was given up as a metastable mess we cleared up by formulating a 'binding' mechanism and showing how to realize equilibrium experimentally.

In our work on the triplet state we were looking at new phenomena in a highly specialized class of systems and the interpretation in terms of quantum theory. We, together with many others, were fascinated at the time, but all we did was explaining details of complex systems in terms of generally accepted theory. Our results were shelved with a lot of molecular spectroscopy but did not lead to any new theoretical concepts.

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

Work with a new (or significantly improved) technique and/or a new type of sample. If you have success and make a significant discovery, you will always be puzzled by further questions. But don't stay with the same system too long. The details may interest only a few specialists and it reduces the probability of chance discoveries.

It may seem efficient to stay with your type of problem, but this is not true. Look around in other fields when you get an opportunity, go to seminars. I picked up new ideas on various occasions. The big hit, of course, was when I went to the colloquium of a (to me) unknown X-ray crystallographer from Oxford, 'Tiny' Powell, who talked on the structure of crystals of rare gases with a mysterious organic compound, quinol. It was a great talk, but I remained with a hidden thermodynamic inconsistency which, years later, made me formulate the proper theory of clathrates.

What is the secret of your longevity, brilliant memory and sharp mind?

For long-levity, I think, one should have the right ancestors; one should have a suitable genetic composition and lead a healthy life. My mother was 99 when she died, and one of her two brothers and a whole set of her uncles became about equally old.

Congratulations to Joan van der Waals round birthday

I wish to address my congratulations to Professor Joan van der Waals and send him greetings from the International EPR(ESR) society.

Edgar Groenen and Jan Schmidt gave a beautiful account on the scientific contributions of Joan van der Waals to molecular spectroscopy; especially optical magnetic resonance and EPR detection of photo-excited triplet states. Therefore, I only want to add some of my own memories on encounters with Joan van der Waals. The first time I meet him was on a '*Hirschegg Rundgespräch*' probably in 1983. I was a diploma student at that time and very impressed about Joan van der Waals *ad-hoc* lecture at this meeting about the importance of symmetry and dynamic Jahn-Teller distortions, which helped a lot to better understand some experimental results presented from other scientists at this meeting. I also remember very much the afternoon hike down from the '*Hohe Ifen*' Mountain, where Dietmar Stehlik decided to take a *direttissima* shortcut along the maximum downhill gradient. This ended with everybody – including Joan van der Waals – sliding down with increasing speed the hill between loose rocks. Fortunately mountain pines stopped all of us at the bottom. Joan van der Waals made some very polite suggestions for the organizers of the next workshop to consider a smoother introduction of Dutch scientists to mountains. Some years later I remember a very nice encounter at one of the famous Amsterdam EPR meetings, where Joan showed us a beautiful teashop. Shortly after, I was very impressed about his way to act as review panel member of a big research grant we defended at the Free University. Where most other reviewers concentrated to talk with the PIs, Joan came to the laboratory and explicitly wanted to talk with us young scientists about details of the proposed projects. My most recent encounter was in spring 2018 at the Joan van der Waals Colloquium at Leiden University. I felt much honored that Joan was not only coming to the talk but also joined us for the dinner and I enjoyed exciting discussion with him as on my first encounter more than 30 years ago! It seems that time has only a rather relative (maybe relativistic) meaning to one of the pioneers of molecular magnetic resonance spectroscopy! Many thanks and all the best for the future, Joan!

Thomas Prisner

It was with great pleasure that I heard of Joan's 100th birthday. He is one of the true gentlemen of science and a man of enormous integrity and distinction. For the younger generation it is often not possible to appreciate what had to be done in order to get the insights that he did. The equipment he used could not be bought but was assembled in Leiden and was unusually innovative. One remembers optically-detected magnetic resonance, a very early Q-band spectrometer, ENDOR spectrometers and pulsed EPR, all developed in Leiden independently of anyone else, although simultaneous breakthroughs were made by Jakob Lebedev in Moscow. They were both great heroes of mine.

Not only did the Leiden group introduce new experimental methods which transformed our understanding of the triplet state in the 1960-70 period especially, but their papers were written quite beautifully and were elegant and perfect examples of how scientific papers should be written.

This is not the place to attempt a review of his scientific contribution, but it is a place to acknowledge his devotion to his many distinguished colleagues and the way in which he encouraged their research.

It has been a privilege and a delight to know him, a man of the highest personal standards.

Keith McLauchlan

Joan van der Waals – 100 years old on 2nd May 2020! All of a sudden it dawned on me[1]

Mel Voet

He may have started the hundredth year of his life, but physicist Joan van der Waals can still be found regularly at the university. Mare, the journal of Leiden University, visited him in honor of his 99th birthday. "The war was like Russian roulette."

"I have to stay active", says Joan van der Waals (99). That is why he does his physical exercises every day diligently: for example, he will walk along the boulevard in Katwijk or Noordwijk. During the past winter, like any other, he returned to the "fascinating void" of Patagonia. He did have to skip his favorite sailing trip across the North Sea for the first time. "More than six months ago, I had to have my hip replaced, without the health insurer complaining."

Van der Waals was a professor of experimental physics at Leiden in the field of molecular physics. He has been Emeritus Professor for thirty years and he turned 99 earlier this month. It does not prevent him from getting on the bus to attend lectures at the faculty, and to start conversations with young and old. Also, he is a distant relative of the famous Nobel laureate J.D. van der Waals.

There is no room for geraniums in his house at the Pieterskerkhof. For M.C. Escher, Chagall and an antique barometer, there is. The house, under the fourteenth-century roof of the former Walloon Library, is officially the oldest building in Leiden, he says. Endless piles of paperwork prevent free passage to his desk. Surrounded by model boats, atlases and encyclopedias, van der Waals draws from a rich memory with playful ease.

"In 1936, the final school exam started on my sixteenth birthday," he says. In Amsterdam, van der Waals was one of the first to receive a Montessori education. "Those teachers were idealists; strict, but very reasonable. You could easily skip a year there." And because he did very well at school, they arranged that for him. A book about Bohr's atomic model that he read with his father sparked his interest in physics. "It fascinated me very much: you could really describe the structure of atoms exactly in a model."

Führer

After an intervening year as a trainee lab technician in London, he started studying physics, mathematics and chemistry at the University of Amsterdam. "That's what it used to be called." He prospered until war broke out shortly after his twentieth birthday. He was a conscript but was released as a prisoner of war "by the generosity of the Führer." He was allowed to continue studying until further notice.

Van der Waals skated the Eleven Cities Tour in 1942. "When I was in Harlingen (about halfway through, ed.) I knew I was going to make it." A year later, like many fellow students, he refused to sign the declaration of loyalty. "A few of my friends were taken away to work in German factories." He was arrested three times himself but managed to stay out of jail. Twice by trying to brazen it out with the Germans, once by running off at an unguarded moment. "When I think about it, it was like Russian roulette."

Towards the end of the occupation, he stayed with family members on the Veluwe. "That region was liberated earlier than the west of the Netherlands." Because he had mastered both German and English, he was recruited as an interpreter. "That was for the Alsos Mission: under the command of Samuel Goudsmit, we had to find out what nuclear weapon knowledge the Germans had passed on to Japan. On board a Canadian army truck I became a co-liberator of the city of Utrecht – an unusual sensation."

Clandestine

During the war he had studied as best he could. "You would do exams surreptitiously, at a professor's home." That allowed him to formally graduate immediately after the liberation. He joined the Royal Shell Laboratory, Amsterdam (KSLA). "Because almost a whole generation of students had dropped out, there was an enormous shortage of people. I was allowed to obtain a doctorate PhD on a subject of my choice at their expense."

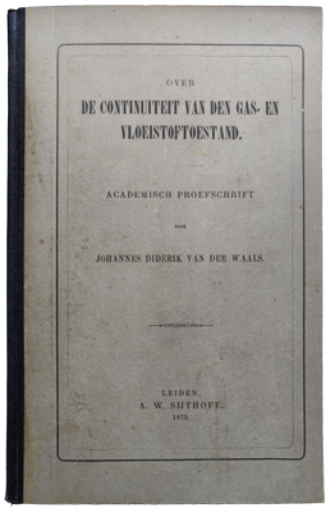
At Shell, he oversaw the lab where the first computer in mainland Europe was located. "That horribly primitive machine gave off a huge amount of heat and was not exactly safe. Back then, computers had electrostatic memories with a sort of television tube element, from which they read tiny surface charges. The input and output went via IBM punch cards. If something happened to those, that was a terrible set-back."

Now, it is almost inconceivable that a mechanical calculator was once regarded as high-tech. "If you previously had to multiply two large numbers yourself, then you pressed the keys of a mechanical hand machine, with gears." As a postdoc in England, six PhD students and van der Waals were "rattling in one room with such a machine". When he became a professor in Leiden in 1967, van der Waals also wanted a table calculator. "You had to get permission for this in The Hague through the ministry, because everyone wanted that."

At the university he focused on spectroscopy and magnetic resonance. Although he did not have to teach, "as that had already ▶

Joan van der Waals with his younger brother, who polishes his army boots, at the start of the war.

[1] https://web.archive.org/web/20190526175900/https://www.mareonline.nl/wetenschap/plots-ging-het-licht-schijnen/ - This article was originally published in Mare, the weekly newspaper of Leiden University (https://www.mareonline.nl/en) on 16th May 2019 just after van der Waals' 99th Birthday. Translated from the Dutch by Robert Kaptein. Editing of translation from the Dutch by John Pilbrow.


OVER
DE CONTINUITEIT VAN DEN GAS- EN VLOEISTOFTOESTAND.
ACADEMISCH PROEFSCHRIFT
JOHANNES DIDERIK VAN DER WAALS.
LEIDEN,
A. W. SIJTHOFF.

Johannes Diderik van der Waals' dissertation.

been taken care of," he could not resist. He started with a rather mathematical lecture on group theory. He is especially proud that "all 25 PhD students have ended up well, their guidance was our first priority." They came en masse, even from China and America, to celebrate his 95th birthday reunion. "A large bunch of them are already retired."

Soldiers' lives

How does he view the current state of science in the hundredth year of his life? "I think it is disgraceful that the NWO (Netherlands Organisation for Scientific Research) requires valorization[2] of your proposed research. Look at the fantastic advances in medicine. There was the work of Mister Röntgen or Mister Fleming. One had showed that you could make an image of someone's skeleton in a strange way, the other was not doing anything medical when he discovered penicillin. This saved many soldiers' lives at the end of the war.

Purcell, a Harvard colleague, once told us in the cafeteria that his team had finally observed magnetic resonance of protons in water. He wondered aloud how the world would benefit from that, but eventually received a Nobel Prize for it." A direct offshoot of that basic research turned out to be indispensable in modern medicine: MRI. Van der Waals also calls it totally irresponsible how the humanities are marginalized. "It absolutely is an essential element in society."

Time for his daily walking exercise. On his way to the smooth boulevard of Katwijk, he will soon have to "cross those terrible bumps of the Nieuwsteeg". On his way, he is sure to pass the grey brigade of onlookers, attached to their motor scooters. Van der Waals has his doubts about it: "you had better exercise".

The Eureka moment

In the fifties, Joan van der Waals caused a furor with his intuitive insights into the description of clathrates and gas hydrates. "These are crystalline substances in which small molecules, and even noble gases, are trapped in a cage by a continuous grid of water, for example." Just before he obtained his doctorate in Groningen, van der Waals attended a startling lecture from Powell, a crystallographer from Oxford, who had also demonstrated similar crystallization of gases such as argon, krypton and methane. "Powell's assumptions about the stability cannot be correct," Van der Waals thought. "It was against the Gibbs phase rule", which ruled it out on thermodynamic grounds.

Van der Waals recalled that "A few years later I attended a lecture in England on solutions of methane in water which lacked an explanation. All of a sudden it dawned on me: you should not see them as chemical compounds, but rather as solutions of the gas. Just as the seawater around Antarctica is stabilized because it contains salt, the crystal lattice in clathrates is stabilised by adding, say, argon. Here too, the molecules have no chemical affinity whatsoever to that water, just like the Van 't Hoff's equation dictates– which explains how diluted solutions behave."

Great-grandfather's cousin received the Nobel Prize

Joan van der Waals is a kinsman of physicist Johannes Diderik van der Waals (1837–1923), who received the Nobel Prize in 1910. "He was my great-grandfather's cousin", says van der Waals. "At the time, he already had four children and often had to go to church. He therefore did the work at home, on the side. While Edison was still discovering incandescent light bulbs and someone else thorium mantles with which you could make good gas light, he wrote his famous work by candlelight and oil lamps."

During World War II, Joan van der Waals took two exams secretly at one of his professors' homes, J.D. van der Waals junior. "Then I was bold enough to ask "Do you still have your father's dissertation?" He said "An aunt of mine just died and a copy turned up there. You can have it." That is now a very rare book that Van der Waals has always managed to keep safe.

[2] Valorization: raise or fix the price or value of (a commodity or currency) by artificial means, especially by government action. It has been used here to indicate that research agencies expect certain outcomes from proposed research.

My love for Magnetic Resonance

Sankaran Subramanian

Indian Institute of Technology Madras, Fellow of the Indian National Science Academy, Fellow of the Indian Academy of Sciences, Fellow of the International EPR (ESR) Society

Professor John Pilbrow (Monash University, Australia), Fellow of the International EPR (ESR) Society [IES] and former IES President suggested that I write an article about the EPR scene in India, soon after I was awarded the 2015 Fellowship of the Society. It was presented to me at the X EFEPR 2016 Conference, Italy on 9th Sept. 2016 by the then IES President Prof. Hitoshi Ohta for which I am very grateful. One of our very senior EPR researchers from India, the late Prof. B. Venkataraman of the Tata Institute of Fundamental Research (TIFR), Bombay who was a pioneer in EPR spectroscopy and instrumentation had already written a chapter entitled "EPR, The Indian Scene" in *Foundations of Modern EPR* edited by Profs. Gareth Eaton, Sandra Eaton and Kev Salikhov, all IES Fellows. That article covers the EPR activities of India till 1997, and Prof. Venkataraman has done such a thorough job that I thought that rather than put the old wine in a new bottle, I shall briefly write about my own journey which led me to the IES Fellowship paying tribute to my mentors and role models and generally reminisce about 50 years of my '*dancing with the electrons and nuclei*'! I had the good fortune of working on EPR (ESR), NMR, MRI and EPR imaging thanks to motivation gained from several stalwarts in magnetic resonance and a bunch of extremely brilliant doctoral students who learned from me and who also taught me much more.

Nevertheless, I should briefly summarize the Indian Scene in the field of magnetic resonance (NMR & EPR). It dawned with Prof. G. Suryan (the name literally means the Sun!) from the Physics Department of the Indian Institute of Science (IISc), Bangalore where he built the first EPR spectrometer with a transmission cavity and diode detection. There were many active groups of spectroscopists across India, and the development of EPR and NMR took off spontaneously right from the 1950s. Professor S. S. Dharmati, who along with J. T. Arnold and M. E. Packard discovered the phenomenon of chemical shift, established NMR research at TIFR, Bombay, and simultaneously A. K. Saha at the Saha Institute of Nuclear Physics, Kolkata. By about the early 1960s many postdocs from USA and Europe were returning to India in search of faculty positions especially in the newly established Indian Institutes of Technology (IITs) at Kharagpur, Delhi, Kanpur, Bombay and Madras. These scholars who returned and established a healthy base for magnetic resonance include Prof. B. Venkatarman (mentored by Prof. G. K. Fraenkel), P. T. Narasimhan (Martin Karplus & Max T. Rogers), P. T. Manoharan (Harry B. Gray & Max T. Rogers) Anil Kumar (Richard Ernst & Kurt Wüthrich), P. Raghunathan (C. A. McDowell) and many others. By about 1970 many advanced technology institutions started procuring NMR and EPR spectrometers and slowly and steadily the field of magnetic resonance started blossoming in India.

B. Venkataraman

P. T. Narasimhan

Among the early stalwarts was Prof. Venkataraman who did pioneer work in the area of EPR hyperfine coupling in π radicals, saturation transfer and relaxation studies and built up the TIFR research group and nurtured it for over three decades. Another was Prof. P. T. Narasimhan who was great at theoretical and instrumentation aspects of magnetic resonance had built up an excellent research school at the IIT Kanpur (one of the first IITs created with the assistance of a consortium of nine US research universities as part of the Kanpur Indo-American Programme). Scientists who came from this school have continued to advance the field of magnetic resonance, some among them being Profs. N. Chandrakumar (IIT Madras), A. Ramamoorthy (University of Michigan, USA), Ravinder Reddy (Perelman School of Medicine, University of Pennsylvania, USA) and many more. A few years later Prof. P. T. Manoharan moved from IIT Kanpur to IIT Madras where I had just joined in 1971, and continued for 25 years till 1996. As for the status of EPR in India, it did not proliferate as well as NMR. The enormous activity in isolating natural products and synthetic organic chemistry oriented several labs to procure NMR spectrometers. EPR was less popular because of the more involved sample preparations as one needs stable free electron systems with narrow resonances. Synthetic transition metal complexes and transition metals (especially Cu^{2+}) doped in diamagnetic lattices were studied by many. Biological applications have been relatively new. The curriculum at the postgraduate level does prescribe EPR spectroscopy, but there is a dearth of qualified teachers in EPR. Even the number of most common X-band EPR spectrometers is small so that in India we need to put in renewed efforts to spread the knowledge and create awareness among the students/scientists the potential and the very powerful applications of this exotic branch of spectroscopy in exploring defects in solids, redox systems, radiation damage, free-radical biology, photochemical and electrochemical redox reactions, transition metal mixed oxides and semiconductors, just to name a few. This was more or less the conclusion of

Prof. Venkataraman, and it has not changed much.

My own journey in Science started with undergraduate and postgraduate degrees from the CMS College, Kottayam (Kerala University, India) during 1958-63. There, Prof. E. T. Matthew, professor of physical chemistry and Head of the Department of Chemistry was the one that motivated me to pursue Chemistry, although I could easily have joined Engineering or Medicine. He was an incredible teacher and educator, who, e.g., will bring a large cucumber to the class room and carve three-dimensional phase diagrams. He was also a great mentor and disciplinarian. After my M.Sc. degree, I joined the Isotopes Division of Bhabha Atomic Research Centre (BARC) Bombay where I learned production of radio isotopes, isotopic labelling, standardization of radioactive sources, production of ^{32}P labelled super phosphate for agricultural research, etc. During my stay at BARC I used to visit the library of the Bombay University Department of Chemical Technology at Matunga for literature survey. I realized that a mere M.Sc. degree is not enough and that I should go for higher studies. I remember, on a Saturday in October 1965, in one of the issues of *Nature*, on the inside back cover was a three-line announcement from Prof. Martyn Christian Raymond Symons, FRS (now IES Fellow), that scholarships were available towards Ph.D. degree at the University of Leicester, UK in Electron Spin Resonance spectroscopy. Without much hope, I wrote an airmail letter (there were no emails, and contacting by phone was next to impossible and very expensive) attaching my CV seeking for admission for Ph.D. Nothing happened for about a month and then one fine morning I received a letter from Prof. Symons that I have been admitted to Ph.D. degree at the Chemistry Department with a scholarship of £ 500 (UK pounds) per annum! It was one of the luckiest days in my life, and I jumped with joy and sent a telegram to Martyn, thanking him and accepting the studentship at Leicester. Thus started my research journey in EPR.

P. T. Manoharan

Anil Kumar

N. Chandrakumar

Martyn Symons

Martyn Symons was a great scientist, highly inspiring and awfully kind to students. He had enormous intuition. He always came up with the correct analysis of complex EPR powder spectra and invariably computer simulation always confirmed his analysis. He published over 800 research papers in subjects ranging from EPR, water structure and solvated electrons, radiation damage, biological EPR, antioxidants, etc. At the time I was in Leicester (1966-68), he was mentoring a bunch of International students (from USA, India, Bangladesh, Australia, Canada, etc.) nearly 20 of them and 6 postdocs. Martyn had an Italian MW engineer, J. A. Brivati who had constructed an X-band EPR spectrometer with a transmission cavity and also a home-built Q-band spectrometer. There was also a Varian V4502 X-band spectrometer in the laboratory with VT accessory. Most of the discussions with students and postdocs took place during the morning coffee-time which used to last for over a couple of hours, all of us sitting around the coffee table with a mug in our hands discussing the latest experiments and results. It was indeed a delightful and highly productive experience. Radiation damage and EPR of trapped radicals were so rich in terms of fail-safe results that everything you touch turns into gold. In about a year and ten months I had already half a dozen publications and enough stuff to write my thesis and so Martyn asked me to write up and submit my thesis. I remember distinctly that when I went to the office of the Registrar, he refused to accept my thesis saying that one cannot submit the thesis before two years are over after registration. So, Martyn suggested I go home to India, come back after 2 months to submit my thesis and offered to support me thereafter as a postdoc for a year. My stay in Leicester was most productive and there were so many discussions with colleagues and postdocs that really expanded my knowledge base. I can never forget Leicester and Martyn for the role they played in my academic life.

I had always wanted to get back to India after Ph.D. for a research/teaching career. During the 2 months gap before submitting my thesis at Leicester, I was called for an interview at TIFR, where Prof. B. Venkataraman was the head of the Chemical Physics group and interviewed me. I was told that I will be given a visiting position and could be regularized after two years depending on my progress/contribution. I was somewhat apprehensive with the title 'Visiting Scientist' and was hesitant to accept, although Prof. Venkataraman did assure me that it was the usual procedure at TIFR. I returned to Leicester in January, 1969 and continued my postdoctoral fellowship to work on transition metal EPR. I also received my Ph.D. degree at the 1969 Leicester University Convocation. My Ph.D. thesis examiner was Prof. C. A. Coulson, the great theoretical chemist and the author of the world famous book Valence. Incidentally, Prof. Coulson was also conferred with the degree of D.Sc. (honoris causa) in the same Convocation in which I received my Ph.D.

Towards the end of 1969 I thought that I would try to do a couple of years of postdoctoral fellowship in the US before returning to India and following up a suggestion from Martyn, applied to Prof. Max Tofield Rogers at the Michigan State University (MSU) with a supporting letter from Martyn. I was promptly offered a fellowship by Prof. Rogers with a stipend of $ 7000 per year, and I became suddenly rich! MSU offered me an independent Married Officers quarters (although I was a bachelor!) and the MSU Credit Union gave me a loan to get a decent car (Pontiac Tempest, I remember) on the first week itself. Being a bachelor and relatively free I spent long hours in the EPR lab where there were Varian X- and Q-band spectrometers, and also the first Varian V-700 ENDOR machine had been ordered and installed very soon. During ▶

my stay at MSU the first 100 MHz pulsed NMR spectrometer from a private company Magnion was purchased and installed. I also travelled a lot excited by a huge car, gasoline at 21 US cents per gallon and four/six lane highways. Max Rogers, who was a Ph.D. student of Prof. Linus Pauling (a two-time Nobel Laureate from California Institute of Technology) was a great mentor, very kind to his students and postdocs and had a great sense of humour. Whenever we discussed a new project within a couple of days all previous literature would be collected by Max T (as we fondly called him), and he would look into the chemicals required and order the same and quietly leave everything on your table. It was indeed flabbergasting to experience such kindness from one's professor. In fact, Prof. P. T. Narasimhan and Prof. P. T. Manoharan who also worked with Max T, have told me about their very similar experiences. After two years at MSU working on radicals/TM ions in single crystals and theoretical open shell calculations of unpaired spin densities, I applied for a faculty position to the IIT Madras and also to Texas Tech at Lubbock. Texas Tech immediately offered me a tenure track position to set up an EPR lab and I was about to accept the offer, when the position of Assistant Professorship was offered to me from IIT Madras in October 1971. At that time there were five IITs in India, all established by an act of parliament as advanced technological institutions and four of them had academic collaboration and faculty exchange link with USA, Germany, UK and Russia. The one in Madras is associated with the Federal Republic of Germany. I accepted the position at IIT Madras and started my faculty career at the Chemistry Department on 1st November, 1971, where already, under an Indo-German Agreement, they had procured a Varian E-4 bench top EPR, a 60 MHz NMR, Perkin Elmer IR, Beckman DU UV-VIS-NIR spectrometer etc. A Special Instruments Laboratory (SIL) was set up as part of Chemistry Department and Prof. P. T. Manoharan who had joined IIT Madras in February, 1972 and Prof. Surjit Singh and myself were put in charge of the lab to provide services to all in the Institute. In 1973 we were jokingly referred to as the 'three musketeers'. We felt that for an advanced institute like the IIT, the analytical and research equipment available for research was rather inadequate and sent out a proposal to the newly formed Department of Science and Technology (DST), Govt. of India requesting grants to set up a sophisticated instrumentation centre, with a promise to maintain them with trained electronic and technical personnel and provide service to anyone from anywhere in India for a nominal charge on a first-come-first-served basis. Professor A. Ramachandran, a former Director of IIT was the first Secretary of DST and he readily approve the project. Thus was born the first Regional Sophisticated Instrumentation Centre (RSIC). We soon added a Varian Laser Raman spectrometer, Varian E-112 X-Q-band EPR spectrometer with Broadline NMR attachment, a Varian XL-100 FT NMR, the first pulse NMR spectrometer in India and a host of state-of-the-art equipment in spectroscopy and analytical chemistry such as TGA, DTA, SEM, TEM, etc.

M. T. Rogers

Surjit Singh

Klaus Möbius

J. R. Pilbrow

In 1976 I had the good fortune of obtaining a short-term DAAD (Deutscher Akademischer Auchtauschdienst) Fellowship and visited the University of Mainz Institute for Physical Chemistry (Prof. H. Sillescu, relaxation in slow motional system and NMR of polymers, 'solid echo', etc.), the Max Planck Institute for Medicinal Research (Prof. K. H. Hausser, a pioneer in electrochemical generation of free radicals and optical detection of magnetic resonance, and Prof. U. Haeberlen, multiple pulse line narrowing NMR) and the Free University of Berlin (Prof. Klaus Möbius, IES Gold Medal and IES Fellow, ultrahigh frequency EPR instrumentation and studies of Photosystem II). Professor Möbuis accommodated me in his own home and treated me like one of the family. This short visit to Berlin and Mainz kindled my interest towards pulsed EPR and NMR spectroscopy.

Our Instrumentation Centre with almost 100% operation of well-maintained sophisticated equipment (we had subsequently added and upgraded much more equipment, electron microscopes, FT-IR, Mössbauer spectrometer, 400 MHz FT NMR with MASS, Mass Spectrometer, etc.) and became a show-case for visitors. The three faculties of RSIC were expanded with the addition of new professors, T. K. K. Srinivasan and Pradeep Thalappil. The five of us at the RSIC organized frequent short-term courses on all branches of spectroscopy with emphasis on magnetic resonance and optical spectroscopy. We had amongst ourselves close to a score of Ph.D. students and half a dozen post docs and the RSIC labs were always humming with activity day and night!

During the winter of 1983 we were visited by Prof. Klaus Möbius under DAAD deputation, who stayed with us for over four weeks. He gave series of lectures on advanced aspects of EPR, pulsed EPR and it was attended by over thirty research scholars. It is during this time that Prof. Möbius who is a great teacher became one of my role models. He enjoyed travelling in India by long distance trains in sleeper cars, I remember. I had had several occasions to meet him over the past 35 years and we always had fond memories to share. Shortly afterwards Prof. John Pilbrow visited IIT Madras during the 1986 Winter Workshop on EPR and gave a complete set of Lectures on Transition Metal EPR. Professor Pilbrow is a great teacher and his book on *Electron Paramagnetic Resonance of Transition Ions* is a Bible for researchers in the field. His group has done tremendous work on dimeric copper complexes as well as generating programs

for their spectral simulation. In the same Workshop Prof. Kees Keijzers (University of Nijmegen, The Netherlands) gave a series of lectures of pulse EPR and ESEEM. I did not have the pleasure of attending these lectures (since I was at NIH on a sabbatical), but I had the pleasure of accessing Prof. Pilbrow's lecture notes which helped me in my teaching at IIT Madras for many years. I also remembered at that time that Prof. Pilbrow had visited MSU in 1971 as a Senior Fulbright Fellow when I was a postdoc with Max T. Rogers, and we had worked on the EPR of high-spin Fe(III) in single crystals of $(NH_4)_2SbF_5$. The work was completed by Prof. Pilbrow's student C. J. Radnel in 1975.

J. Chandrasekhar

In my 25 years of academic life at IIT Madras I had the good fortune of getting very bright students who would finish their M.Sc. degree there themselves and then would want to work for Ph.D. in our Centre because of the excellent facilities for spectroscopic research and the availability of fast computers in the institute. My first Ph.D. student Dr. J. Chandrasekhar was a rank holder throughout his studies and started working on EPR of transition metals. His first work was on Cu(II) under axially compressed Oh environment for which he hunted and chose the lattice of $(NH_4)_2[Zn(NH_3)_2(CrO_4]_2$. He was, however, more interested in developing novel non-empirical quantum mechanical calculations and with my colleague Prof. P. T. Manoharan and a fellow student P. K. Melhotra developed the NDDO MO calculations. He was brilliant and quite successful, continued doing postdoctoral fellowship with Prof. Paul von Ragué Schleyer (University Erlangen-Nuremburg, Germany), and interacted with the Nobel Laureates John Pople, H. C. Brown, R. Hoffmann and G. A. Olah. He returned to India as Chemistry faculty at the IISc Bangalore. He also received the Citation Laureate Award of Thomson Scientific for the most cited scientist in 2004. Prof. Chandrasekhar now works as chief scientist developing computer-based drugs for Gilead Sciences, USA.

I have guided more than 20 Ph.D. students, all of whom without exception, are pursuing research in magnetic resonance (EPR/NMR) with the exception of one guy, Dr. Dinesh Nettar who was so good in computational skills and mathematics that his part-time job during his graduate studies was to guide mathematics and computer science graduate students! Nevertheless, he produced a wonderful thesis in EPR, and the external examiner from USA wrote that this was the only thesis in which he could not find any mistakes both EPR-wise and the English language syntax was flawless. My Ph.D. students worked in the areas of EPR, pulse NMR and theoretical calculations. All of them, without exception, were brilliant and therefore I learnt much more from them than what I gave!

While at IIT there was a visit to our Department, I believe in 1974, by Dr. Edwin Becker (Laboratory of Chemical Physics, NIDDK) and Director of Research Services (NIH, Bethesda USA). He was an expert in vibrational spectroscopy and NMR and was behind the developments of biomolecular NMR and in vivo MR imaging research and development at NIH. He was also the chief of IUPAC. He gave a scintillating talk in pulsed NMR. In order to explain the free induction decay (FID) he had mixed the damped oscillatory frequency down to audio region and the audience could 'listen' to it as decaying monochromatic sound, and in the case of multiple frequencies one could listen to decaying beat patterns. After listening to Dr. Becker, I decided that I should learn the tricks of NMR, as after all, it is not much different from EPR, basically.

Dinesh Nettar

The chance to dabble in NMR came in 1979 as a fellowship from the Alexander von Humboldt (AvH) Foundation to work with Prof. H. Sillescu (University of Mainz, Germany), with whom I had spent a short time in 1976 with a DAAD fellowship. I was given the opportunity to design a Hartmann-Hahn double resonance probe for rotating frame cross polarization from proton to ^{13}C at 300 and 75 MHz, respectively. At that time there were no commercial double resonance probes and it was a challenge. By getting a lot of help from Dr. Hans Wolfgang Spiess (Sillescu's group) and gifting some crates of beer for the workshop gentlemen I got the probe fabricated with quartz-tube/brass plunger capacitors, and ended up getting a functioning doubly tuned Hartmann-Hahn rotating frame polarization single-coil resonator which actually worked. I also worked on spin lattice relaxation of concentrated polymer solutions. The AvH Foundation made our stay very comfortable making it possible to learn rudimentary German language, travel in Germany and make a lot of long-lasting friends.

In the mid-eighties my former Ms.D. student Dr. N. Chandrakumar had returned to Madras after his Ph.D. at IIT Kanpur, to set up an NMR research lab at the CSIR-Central Leather Research Institute right across from IIT campus. We met frequently to discuss pulse NMR and in particular the coherence transfer phenomenon. Dr. Chandrakumar is an expert in the density matrix treatment of NMR and I have learnt a lot from him. We also attended many delightful lectures in high-resolution NMR by the Nobel Laureate Richard Ernst (ETH Zurich, Switzerland). During several of our discussions we felt the need to describe the entire NMR on a monolithic density operator formalism and ventured upon to write a book. When we contacted Prof. Ekkehard Fluck (Gmelin-Institut, Frankfurt), one of the editors of Springer series, "NMR: Basic Principles and Progress" with a synopsis for the book. Professor Fluck readily agreed and encouraged us to go ahead with the writing of the book. Springer-Verlag New York took up the publishing of our book entitled

Edwin D. Becker

Hans Sillescu

Richard Ernst

Murali Krishna

"Modern Techniques in High Resolution FT-NMR" which was released in 1987 and was appreciated highly by many NMR stalwarts including Profs. Richard Ernst, Ray Freeman (Cambridge University, UK), Dieter Ziessow (TU Berlin, Germany). Dr. Chandrakumar joined IIT Madras in 2001 and is a Chair Professor and is working on several aspects of NMR, namely coherence transfer, MR imaging, EPR imaging and dynamic nuclear polarization.

The opportunity to work on high-resolution multi-dimensional NMR and coherence transfer based two-dimensional spectroscopy came in 1985 when Dr. Edwin Becker of NIH offered me a Visiting Scientist position to work with Adrian Bax when I spent a sabbatical year there. We developed some very useful sequences to separate and generate sub spectra of individual sugar units from polysaccharides using homonuclear Hartmann-Hahn transfer (HOHAHA), known also as 'isotropic mixing' and also designed a pulse sequence for sensitivity enhanced heteronuclear ^{13}C-^{1}H 2D correlation spectroscopy using inverse detection. It was a very profitable time research wise, and I could learn the nitty-gritty details of high-resolution pulse NMR.

During my stay at NIH, one of my IIT Madras graduate students, Dr. Murali Krishna Cherukuri (2015 IES Silver Medal in Biology/Medicine) was working at the Radiation Oncology Branch with Dr. Peter Riesz on the generation of free radicals by ultrasound, stabilizing them using spin traps. He was also involved in the application of CW EPR to assess tissue redox status using stable nitroxides. It was during my stay at NIH that on one of the lunch-breaks Dr. Angelo Russo from the Radiation Oncology Branch asked me, "I understand MRI, but can we do similar imaging with unpaired electrons?". We noted that already using L-band (1-2 GHz) CW EPR and stable nitroxides filtered back-projection in presence of linear gradients have been used to generate phantom and small animal imaging. CW EPR imaging and oximetry have been carried out at Johns Hopkins University by Prof. Jay Zweier and Dr. Periannan Kuppusamy (former Ph.D. student of my colleague Prof. P. T. Manoharan), and spatially resolved nitroxide and fusinite images were practised in Italy, Belgium and USA. But pulsed EPR imaging was not routine. In fact, most of CW EPR imaging practices and the so-called spectral-spatial imaging which addresses the real spatial dimension and a virtual spectral dimension had been perfected by several groups including Profs. S. Eaton and G. Eaton, H. Utsumi, M. Alecci and A. Sotgiu, M. M. Maltempo and many others. A book entitled *EPR imaging and in Vivo EPR* edited by the Eatons and Prof. Keichi Ohno is a comprehensive source on the subject up till 1990. The importance of in vivo EPR imaging arises from the fact that the line widths of most EPR probes are linearly dependent on the oxygen concentration and it should be possible to map out the oxygen distribution in tissue non-invasively by linewidth-weighed EPR imaging. Besides it was well known that hypoxic zones (tissue pO_2 less than 5 mm of Hg) observed in most tumors make them highly radiation-resistant (nearly 4-fold). Non-invasive oxygen mapping will thus help in programmed radiation dosing and improve the efficiency of cancer therapy. Dr. Murali Krishna and I decided to embark on the development of pulsed EPR imaging knowing very little the great challenges to be faced.

I took a sabbatical in 1993 and arrived at the National Cancer Institute (NCI), Radiation Oncology Branch. With the solid support of Chief Dr. James Mitchell, and colleagues Drs. Angelo Russo and Murali Krishna we embarked on the development of pulsed EPR imaging for in vivo applications. First, we decided that the frequency of imaging should be around 300 MHz to facilitate tissue penetration. Lowering the frequency brings down the sensitivity roughly as $(\text{frequency})^{2.5}$. Further we did not realize that even at very low pulse power the dead-time in the case of stable nitroxide-type free radicals will be an order of magnitude larger than T_2 and hence there would be no way of capturing the FID! Therefore we needed to use pulses of 50–100 ns duration. The very fast decay would entail ultra-fast digitization requirements and compatible A to D converters with more than 10 MS/s and these were not commercially available. Mr. Rolf Tschudin, an expert in MW and RF instrumentation who was working at the Laboratory of Chemical Physics in the Research Group of Dr. Ted Becker and Ad Bax helped us make resonator coils, band pass filters and many required components. In spite of damping the quality factor Q of the resonator to less than 20 we never could see the FID. It suddenly dawned upon us that solvated electron in liquid ammonia had a long relaxation time (several microseconds) and we decided to start the exploration with samples of sodium dissolved in liquid ammonia under sealed vacuum. Drs. Angelo Russo and John Cook helped us enthusiastically in getting the required chemicals, vacuum lines and ammonia cylinders. When we were struggling to procure a fast A to D converter, Walter Friauf and Thomas Pohida of the NIH Biomedical Engineering and Instrumentation Programme Division designed and constructed 250 MS/s 8-bit A to D converter. Using a home-built 106 G (10.6 mT) electromagnet with coils wound on a Lucite cylinder, we could monitor the FIDs from solvated electrons. Very soon we were able to procure a Tektronics 500 MHz oscilloscope and using a home-built gradient coil system we could image tubes of solvated electrons using 2D gradients and filtered back-projection. The data acquisition and computational help was provided by our colleague John Bourg. The manuscript was sent to JMR in July 1993 and got published in the August issue JMR series B, volume 102, issue 01. It was reviewed by the Chief Editor Prof. Wallace Brey and accepted right away.

Since the highly unstable and reactive solvated electron is not a suitable probe for in vivo applications, we were looking for biocompatible narrow-line spin probes. While Fusinite (derived from coal) is a stable non-toxic implantable in vivo spin probe, it had line widths not suitable for time-domain EPR. By then lithium phthalocyanine (LiPc) was found to be a narrow-line EPR spin probe with an extremely narrow line width and a large linear linewidth dependence on pO_2, and we embarked on the electrochemical synthesis of LiPc and were able to use it to monitor in vivo pO_2 focally at the implanted site in mice using FT EPR. My sabbatical ended, and I was able to enthuse another one of my Ph.D. students Prof. Ram Murugesan to continue the imaging work at NIH and he made substantial improvements. After I returned

to India, the Radiation Biology chief Dr. James Mitchell, and colleagues Drs. Angelo Russo and Murali Krishna used to call me (invariably at past midnight because of the time difference!) several times saying that we have to carry forward the FT-EPR imaging further to animal models and to explore the impact of FT-EPR imaging in radiation oncology and cancer research. Convinced that it is important to continue further advancement of FT-EPR imaging I took voluntary retirement from my position at IIT Madras and joined as visiting scientist at NCI, Radiation Biology Branch in 1996 with Murali Krishna, my former Ph.D. student and the Principal Investigator of Biomedical Spectroscopy and Imaging.

R. Murugesanj

A. W. Overhauser

N. Devasahayam

Murali Krishna, who keeps excellent track of literature and had been on the lookout for biocompatible water-soluble spin probes, came across the series of patented triarylmethyl derivatives from Nycomed Innovation AB, Malmö, Sweden. These are now marketed by GE Healthcare. Nycomed developed these compounds to perform Overhauser enhanced MR imaging (OMRI) by transferring polarization from unpaired electrons to protons. The technique which was developed in parallel by Prof. David Lurie at Aberdeen was called PEDRI (Proton-Electron Double-Resonance Imaging). Since the Overhauser transfer depends on among other things the linewidth of the electrons which in turn depends on pO_2 Jan-Henrik Larsen and Klaes Golman et al. of Nycomed Innovation were using OMRI for oximetry as well as low field MR imaging and angiography in animal models. Dr. Murali Krishna saw a great promise for EPR imaging in getting our hands on to these exotic spin probes and was able to convince Prof. Golman of Nycomed to give us a small quantity of the spin probe Oxo63. With Nycomed's help we also signed a CRADA (Cooperative Research and Development Agreement) with Philips Medical systems, Hamburg to fabricate an Overhauser imager where we could do in vivo MRI and oximetry on mice and rat tumor models at very low fields as a complement to our own direct EPR based oximetry. We succeeded in performing OMRI based oximetry and had the pleasure of a visit by Prof. Albert W. Overhauser from Purdue University, W. Lafayette who was thrilled to note that his discovery of dynamic nuclear polarization was now being used in life sciences and cancer research.

By this time, we also had encouraged Mr. Nallathamby Devasahayam, an electronics expert trained by the German engineers at IIT Madras to join the NIH team to help with developing resonators and RF instrument design. Our early imaging of mouse tumors was based on infusion of Nycomed compound into mice via tail-vein cannulation followed by spatial encoding with gradients and image reconstruction via filtered back-projection. We could get excellent oximetric images that could be corroborated with direct Eppendorf polarographic electrode measurements. Both T_2^* weighted images and T_2 weighted images were initially used for oximetry, but the images suffered limited resolution due to gradient-induced line-broadening. During one of the presentations at the International Workshop on Techniques and Bio-Medical Applications of In Vivo EPR and PEDRI at Aberdeen, Scotland in 1999, we had a casual discussion with Dr. Joost Lohman of Bruker, UK who suggested that one can try EPR imaging using constant-time phase-encoding to avoid linewidth dependence on resolution and to circumvent deadtime problems. As soon as we got back to NIH we started working on sequences to generate constant-time (single point in the FID) with pure phase encoding on all dimensions that generated 2D and 3D images that were by far the best we have seen anywhere in the literature. We could introduce the relaxation weighting by phase encoding a series of delayed time points and after suitable scaling (single point images will have a zoom-in effect as a function of delay from the pulse). We could introduce relaxation weighting. This was our best and fast mode of oximetry which helped us perform oximetry in many mouse tumour models with mm resolution both in spatial dimension and pO_2 dimension. I was awarded the first IES Silver Medal for EPR instrumentation in 2000. It was presented to me by Prof. John Pilbrow at the Rocky Mountain Conference in 2002.

The quality, reproducibility and the resolution of single point Images in vivo were so good that we decided to perform co-registration of MRI and EPRI which was straightforward since our measurement frequency was 300 MHz, and many MR animal imagers (e.g., Bruker and Siemens) operate in the same frequency. We have had the pleasure of a number of brilliant hardworking Japanese postdocs, Drs. Ken Ichiro Matsumoto, Atsuko Matsumoto, Shingo Matsumoto and Fuminori Hyodo who had contributed in a big way to perform MRI-EPRI co-registration, and NCI established itself as the leading functional EPR imaging centre. In spite of all the productivity in EPR oximetry there was one thing that still requires more looking into, namely the FDA limits of SAR (specific absorption rate) in imaging because for scaling up the EPR oximetric imaging at least for surface tumors, it is clear that using 40–50 ns pulses at 200–500 W power even with a duty cycle of 1% could exceed the prescribed FDA limits for human measurements. Towards achieving admissible SAR for human imaging we have developed a rapid scan imaging strategy (which has been patented) using a low power (~mW) CW imager at 300 MHz employing rotating space encoding gradients and sinusoidal Zeeman sweeps both employed simultaneously. The resulting projections are unravelled mathematically into regular projection profiles and images could be generated very rapidly in a matter of minutes at very low power. Crossed resonators and DSP based instrumentation are being developed by the team at NCI, namely Dr. Murali Krishna, Mr. Nallathamby Devasahyam, Randall Pursley, Thomas Pohida and Janus Koscielniak. Proof of the principal correlation methods have also been developed to reduce SAR in pulsed mode using 'spread spectrum' sequences like Frank phase-chirped sequences, as well as stochastic excitation using Hadamard pseudo-random

phase sequences. All these contributions were made possible by inspiring mentors, excellent co-workers, and the friendly and invigorating work atmosphere at NIH. Incidentally, two of our own students Prof. P. Kuppusamy (currently at Dartmouth Medical School) and Prof. Murali Krishna (NIH) were elected as Distinguished Alumni of IIT Madras, the former for CW EPR imaging and oximetry and the latter for FT EPR imaging oximetry and cancer research.

I returned to my Institution, IIT Madras, in 2015 and was made Adjunct Professor at the Chemistry Department, and am occupying the same room that I occupied when I was the Chairperson of the Regional Sophisticated Instrumentation Centre during 1980-85 and 1990-95! I continue to teach magnetic resonance at various institutions via short-term courses. I am currently the President of the National Magnetic Resonance Society (India). Recently with funding from the Department of Science and Technology under the Global Initiative of Academic Networks (GIAN) I, along with Prof. Thomas Prisner (BMRC, Goethe University Frankfurt am Main and the current IES President) had the pleasure of conducting a two-weeks' school on "The Principle and Applications of Electron Paramagnetic Resonance Spectroscopy", (29 Jan. – 9 Feb. 2018) at the National Institute of Technology, Goa hosted by Prof. Velavan Kathivel, a Ph.D. student of my former Ph.D. student, late Prof. P. Sambasiva Rao (ex HOD, Pondicherry University).

I owe whatever little I have achieved and contributed in my academic career to ALL MY ESTEEMED TEACHERS, ROLE MODELS, MY BRILLIANT STUDENTS AND CO-WORKERS to whom I dedicate this write up. I sincerely thank Professor John Pilbrow who requested me to write something about EPR and I took the liberty of writing about my journey through magnetic resonance for which I may kindly be excused.

I sincerely thank Dr. Laila Mosina, Editor of the EPR newsletter, for having been very patient and providing all the moral support. Last, but not the least, I thank my better-half Rajalakshmi Subramanian, for putting up with me, a crazy scientist, taking care of me and cooking for me the most healthy and tasty gourmet vegetarian food, that means I never have to watch my weight!!

Dale Pace (1952–2020)

It is with deep sadness that Balaraman (Raman) Kalyanaraman (Medical College of Wisconsin, USA) shares the passing on September 2, 2020 of a friend and colleague, Dale Pace, following a two-year battle with ALS. Dale took a sabbatical in the Department of Biophysics at the Medical College of Wisconsin in the early 1990s, working with Jim Hyde and Teddy Christidis, which resulted in the publication of two papers (Pace MD, Christidis TC, Hyde JS. S-Band ENDOR of Hyperfine Interactions of ^{1}H and ^{14}N Nuclei in Trinitrophenylmethylnitroxide. J Magn Reson

102A: 101-104, 1993; Pace MD, Kalyanaraman B. Spin trapping of nitrogen dioxide radical from photolytic decomposition of nitramines. Free Radic Biol Med 15: 337-42, 1993). Dale earned his BS, and under the direction of Lowell Kispert, his PhD, from University of Alabama. He later joined the Naval Research Lab where he worked on the role of free radical degradation in explosives, and published the book, FILMCAL: An ESR (Electron Spin Resonance) Simulation Program for Transition Metals in Phthalocyanine Films. Dale became interested in low-temperature EPR, ELDOR and ENDOR, and was a regular attendee at the EPR Symposium of the Rocky Mountain Conference. He taught chemistry at Bevill State Community College in Jasper, Alabama for many years. Dale will be missed for his friendship and quiet sense of humor.

The 58th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2019)

November 7–9, 2019, Tokyo, Japan

The 58th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2019) of Japan was held in Kawasaki City Convention Hall, near Tokyo in November 7–9, 2019. This annual meeting was jointly organized with the 58th annual meeting of the NMR society of Japan (Chaired by Dr. Takanori Kikawa, Group leader, Institute of Physical and Chemical Research, Yokohama). Both societies are committing to support ISMAR-APNMR2021 meeting, which is scheduled to be held in Osaka, Japan in 2021. This joint meeting of SEST2019 and 58th NMR meeting was a valuable occasion for the future cooperation of the two academic societies for ISMAR-APNMR2021.

At the joint meeting, each society was basically held independently, but we set the same period and venue, so that we could organize joint sessions, make mutual auditions possible, and hold social gatherings together. The number of participants at the SEST2019 was 165 and total number including the NMR meeting was about 500. The oral lectures were given at the parallel sessions with NMR meeting, and the joint sessions were given at the same venue. We had joint session for a few hours a day and 9 invited talks were presented to argue the common interests of both society members. In the SEST2019, two society award lectures and three young investigator award lectures were given in the afternoon of the second day, before the conference banquet. The number of general talks was 48 at the SEST oral session hall. The poster session of 56 presentations from SEST2019 was held jointly with NMR meeting. The corner of the sponsored company was set up using a foyer jointly with the NMR side, and we were able to introduce information of about 20 companies.

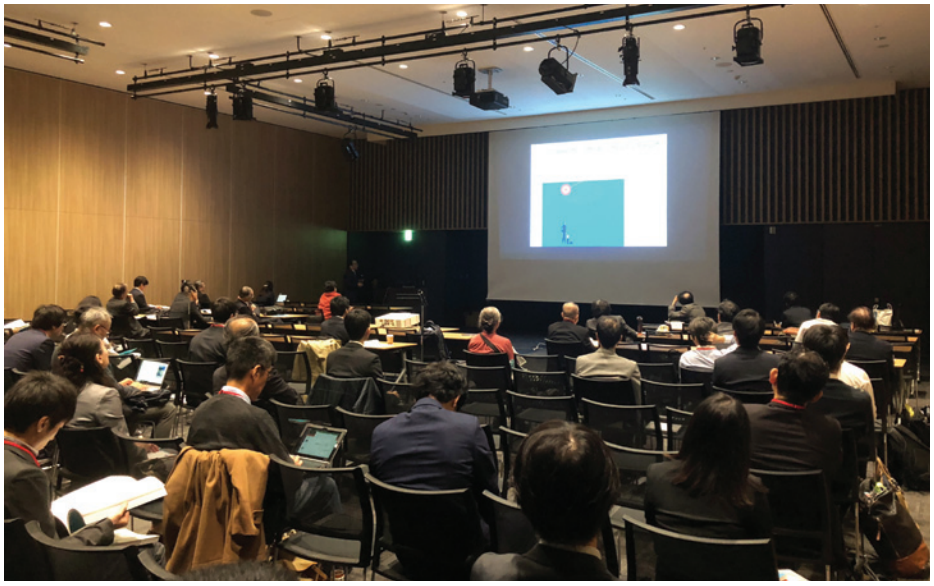
November 7th The morning oral session of the first day in the SEST2019 was for young participants who were nominated for an excellent lecture Award of young investigators. General lectures (Solid-state electronic properties) were subsequently held. After lunch, the first joint session with NMR meeting was held, and four invited lectures were given on the theme of "Electron Spin and Nuclear Spin Concertation-Dynamic Nuclear Polarization (DNP)" hosted by the NMR side. After that, a poster session was held jointly. After the poster session, other general lectures (Biochemistry using ESR) were given and the program of the day was completed. In the evening, SEST Young People's Association and SEST Committee Meeting were held at the conference venue.

November 8th The morning session of the second day, was started with a joint session hosted by the SEST side. Under the title of "Spin Polarization Generation and Magnetic Resonance Measurement Using Light", lectures and discussions on light-induced dynamic electron spin phenomena were made with a view to develop methods for generating nuclear spin polarization by photoexcitation of the chemical matters. In this session, Professor Chris Wedge (UK) and Professor Chris Kay (Germany) were invited from abroad, and Professor Kiminori Maeda (Saitama University) from Japan gave an invited lecture. A joint session in the morning was followed by a related general session (Spin dynamics) including two invited lectures until lunch break. The official language of this morning sessions were English although SEST annual meeting is domestic.

In the afternoon, a SEST member meeting was held, including activity reports, financial reports, award ceremony for SEST Society Awards, Young investigator Awards, and new honorary members. Professor Toshiaki Arata (Osaka City University) and Professor Toshimichi Fujiwara (Osaka University) received the Society Awards of 2019. Dr. Kenji Sugisaki (Osaka City University), Dr. Hideyuki Takahashi (Kobe University), and Dr. Yusuke Miyake (Kyoto Institute of Technology) received Young investigator Awards 2019. In addition, Professor Hisao Murai (Shizuoka University) was newly elected as an honorary member of SEST. In the end of SEST member meeting, a venue of the next SEST2020 in Kumamoto city center was introduced. After the member meeting, prize-winning lectures from five honorable members were given. The titles of the talks were as follows.

Professor Toshiaki Arata: "Exploring the principle of protein operation using advanced spin label ESR"

SEST Society Awards (upper): From left to right: Prof. Toshimichi Fujiwara, SEST President, Prof. Kunihiko Tajima, and Prof. Toshiaki Arata.
Young investigator Awards (lower): From left to right: Dr. Kenji Sugizaki, SEST President, Prof. Kunihiko Tajima, Dr. Hideyuki Takahashi, and Dr. Yusuke Miyake.



Oral session hall.

Professor Toshimichi Fujiwara: "Development of high-sensitivity and high-resolution solid-state nuclear magnetic resonance experimental method using high-field dynamic nuclear polarization using electron spin polarization"

Dr. Kenji Sugizaki: "Development of quantum chemical calculation method and quantum computer quantum algorithm for magnetic properties of high spin open shell system"

Dr. Hideyuki Takahashi: "Development of Force Detection Electron Spin Resonance Method in Terahertz Region Using Nanomembrane"

Dr. Yusuke Miyake: "Molecular study of physical properties and formation mechanism of functional molecules by ESR spectroscopy"

After the award lecture, a conference banquet was held at the Hotel Seiyoken, a 10- minute walk from the conference site. SEST2019 and NMR meeting participants joined together.

November 9th Third day was started with three general lecture sessions (Recombination in the excited state, functional materials, equipment development and biomedical applications). In the afternoon, third joint session was organized with a theme of the three-dimensional structure analysis of protein by both ESR and NMR. In this session, there were two invited lectures, one from SEST and the other from NMR meeting. After that, there were general lectures about the topics, Electronic States and Reaction Mechanisms. Then, SEST2019 was concluded with the closing remarks from SEST President, Professor Kunihiko Tajima.

The day before SEST2019, the ESR Users Forum, which started last year by SEST council, was held at Kanagawa University, Yokohama Campus. Professor K. Tajima, who was the president of SEST, was a chairman of the forum, and we received participation mainly from members of the company researchers. At the forum, there were many tutorial lectures concerning ESR apparatus, spectral analysis and some related practical aspects of ESR spectroscopy.

In 2020, SEST was supposed to have an annual meeting in early November in Kumamoto, Kyushu area of Japan. However, because of the present COVID-19 pandemic, we recently changed annual meeting schedule. SEST annual meeting will be held in November 13–15, 2020 as a web meeting organized by Professor Hiroyuki Nojiri from Tohoku University, the vice president of SEST.

Very recently it is decided that SEST2021 headed by Professor Akimoto, Wakayama University, Japan, will be held on line at the end of Aug. (tentative) following the on line conference of ISMAR-APNMR2021 headed by the team of Professor T. Fujiwara, Osaka University, Japan.

Finally, I would like to thank the members of the NMR Symposium Executive Committee for their support for the Alliance on the occasion of the two annual meetings.

Akio Kawai, Chair, SEST 2019
Professor, Department of Chemistry,
Faculty of Science,
Kanagawa University, Japan

Jason W. Sidabras

Jason Sidabras will become an Assistant Professor of Biophysics at the Medical College of Wisconsin (USA) in December 2020. Dr. Sidabras received his BS in Electrical Engineering Technology in 2003 from the Milwaukee School of Engineering (USA) and his MS in Electrical Engineering in 2010 from Marquette University (USA). He worked as a Research Engineer in the lab of Prof. James S. Hyde at the Medical College of Wisconsin from 2003–2016 where he developed innovative EPR and MRI probes for frequencies ranging from 250 MHz to 260 GHz. Dr. Sidabras completed his PhD in Physics in 2020 at the Technische Universität Dortmund (Germany) as a Marie Skłodowska-Curie Actions Fellow (Act-EPR; EU Horizon 2020 grant) within the Max Planck Institute for Chemical Energy Conversion under the direction of Profs. Wolfgang Lubitz and Dieter Suter. During this time, he developed resonators to study protein single crystals of limited dimensions (less than 0.3 mm) and applied this technology to determining the full g-tensor of the [FeFe]-hydrogenase active site (Hox state). This work led to the 2019–2020 IES best paper Award (DOI: 10.1126/sciadv.aay1394). Additionally, he has been honored with the JEOL Young Investigator Award (ISMAR2017) and the Young Investigator Award for Outstanding Oral Presentation at EPR2017. His independent research will focus on advancing the state-of-the-art in magnetic resonance instrumentation to improve sensitivity to study both structural and functional enzymatic activity.

IES Virtual EPR Meeting
May 08, 2020

Role of EPR Detection in Deciphering DNP Mechanisms

Asif Equbal,
Han Lab, Department of Chemistry and Biochemistry, University of California Santa Barbara, Santa Barbara, CA, 93106-0520 USA

Dynamic Nuclear Polarization (DNP) is revolutionizing NMR spectroscopy and imaging by boosting its sensitivity by several orders of magnitudes. DNP uses microwave irradiation to transfer large electron spin polarization to nuclear-spins [1]. There are four general DNP mechanisms: Overhauser Effect (OE), Solid Effect (SE), Cross Effect (CE) and Thermal Mixing (TM) [2]. This classification is based on the number of participating coupled electron spins and their dynamics under microwave. OE requires hyperfine dynamics driven electron-nucleus cross-relaxation, and therefore is normally not anticipated as an effective mechanism in insulating solid-samples. SE is practically inefficient at high magnetic-fields (above 5 T) because it requires high-power microwave irradiation, a limiting factor with state-of-art instrumentation. The most efficient DNP mechanisms such as CE and TM involve coupled electron spins. In these mechanisms triple-flip of two coupled electron spins and a nuclear-spin, achieved when the frequency difference of the two electron spins matches the nuclear Larmor frequency, drives the polarization transfer.

In spite of tremendous development over the last two decades, the experimental efficiency of DNP is still far below the theoretical maximum. Recognizing the DNP mechanism is indispensable. This is because the design principle for the optimal polarizing agent or PA (unpaired electron spin), the DNP instrument, microwave pulse sequence and experimental conditions are entirely different for different DNP mechanisms. With the incorrect or incomplete understanding of DNP mechanism, its translation to application is stymied. A lack of insight into the electron spin dynamics is the bottleneck [3].

Recently, we reported on a surprising, but fundamentally important, observation in ^{1}H DNP using Trityl-OX063 which is one of the most widely used PAs for biomedical NMR applications. The dominant DNP mechanism crossed over from the expected SE to the unexpected TM-DNP with increasing PA concentration. The discovery is highly important as the TM-DNP mechanism increased the DNP efficiency by 4x compared to SE, while dramatically lowering the microwave power requirement [4].

EPR detection played a critical role in confirming the existence of TM-DNP mechanism. Using a home-built 7 T dual EPR-NMR spectrometer developed in the Songi-Han-Lab at UC Santa Barbara [5, 6], we examined the electron spin dynamics under DNP operating conditions, and discovered characteristic EPR signatures that corroborated the theoretical prediction of TM-DNP. Firstly, asymmetry in the case of a primarily dipolar broadened EPR line was ascertained as quantum mechanically predicted by Water Kockenberger and coworkers at Nottingham [7]. Asymmetry helps in maintaining a large polarization gradient under microwave irradiation and thus induces a large DNP enhancement [8]. Secondly, a significant hyperpolarization of strongly coupled electron spin populations in pump-probe ELDOR [9] experiments was observed. This confirms the theoretical prediction of TM-DNP made by Shimon Vega and coworkers [10]. Notably, hyperpolarization (also termed as "anti-hole") has also been used for investigating electron spin proximity in Cu(II)-porphyrin dimers by Jeschke and coworkers[11].

Using a powerful EPR-toolbox, we ascertained that TM DNP is the dominant mechanism even in concentrated BDPA radicals; this system has caught immense interest by the DNP community given its promising DNP performance at high magnetic-field, under fast magic-angle spinning conditions and at higher temperature, i.e. the desired experimental conditions for bio-solid NMR [12]. Our research emphasizes the need to investigate electron spins dynamics properties via EPR under DNP conditions to gain an in-depth understanding of the underlying DNP mechanisms, and in turn to push the limits of the (experimentally) achievable DNP enhancement closer to the theoretical limit. In particular, EPR measurements to access EPR line-shape, electron spin-lattice and spin-spin relaxation rates and electron-spectral-diffusion are critical to discern and fine-tune the role of electron spins in DNP mechanisms. This in turn can lead to discovery of new territories in DNP.

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VI International School for Young Scientists: Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics: Virtual Event
September 2–10, 2020

http://roshchino2020.tomo.nsc.ru

The 6th International School for Young Scientists "Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics" was held on 2–10 of September as a virtual event. Originally planned as a meeting in Roshchino (St. Petersburg region, Russia), the school with physical presence had to be abandoned due to COVID-19 issues, but the organizing committee had decided to proceed in online format. This did bring some advantages, especially in terms of cutting the expenses for both the organizers and the participants as all problems related to travel

and visas were eliminated, but these were more than compensated by the challenges and problems related to the virtual nature of the event. The main difficulties were related to communication problems introduced by the online format, and time differences between home countries of the participants and therefore limited duration of scientific sessions. As it was hardly realistic to keep attention of students for longer than 4 hours per day, the School was split into two parts: 6 introductory lectures on 2–4 September were followed by the main school on September 6–10, for a total of 9 day long virtual meeting.

The teaching program comprised 15 lectures, starting with 6 introductory lectures to have the grounds firmly covered, followed by 9 lectures on various NMR and EPR subjects during the main School, with ample time for discussions and a virtual tutorial. To stimulate active participation of the students, 6 virtual poster sessions with short "poster talks" delivered by students were organized. The teachers of this School were Danila Barskiy (Berkeley), Christian Griesinger (Göttingen), Konstantin Ivanov (Novosibirsk), Leonid Kulik (Novosibirsk), Olivier Lafon (Lille), P. K. Madhu (Hyderabad), Kiminori Maeda (Saitama), Valentin Novikov (Moscow), Kev Salikhov (Kazan), Takuya Segawa (Zurich), Hans-Martin Vieth (Berlin), and Maxim Yulikov (Zurich).

The students were asked to make a self-presentation by introducing themselves and briefly explaining their area of research, in order to ease communication and compensate partly for the inability to meet in person. The tone was set by the self-introduction of the organizers and teachers, and the three "introduce yourself" sessions really helped establish the contact despite thousands of miles separating School participants. There have been 81 students from 16 countries, 42 students have presented their work during the virtual poster sessions. Six "best poster" prizes were awarded to: Arnau Bertran (Oxford, UK), Giuseppina Magri (Cardiff, UK), Natalya Sannikova (Novosibirsk, Russia), Fabio Santanni (Florence, Italy), Taichi Sato (Saitama, Japan), and Agnes Thorarinsdottir (Cambridge, MA, USA). A special prize of the organizing committee was awarded to Georges Menzildjian (Lyon, France) for his scientific contribution and active work during the School.

From left to right: Leonid Kulik, Konstantin Ivanov, and Dmitri Stass.
Photo taken by Dr. Olga Morozova, ITC SB RAS.

The organizing committee had raised funding from several sources, including Groupement AMPERE, ISMAR, Humboldt Foundation, Russian Science Foundation and Wiley, planning for the physical presence event. However, the meeting has turned out to be very inexpensive, and the secured funds were not claimed: the only costs were prizes to students (Wiley books, 7 prizes in total). Nonetheless, the organizers are grateful to all organizations that agreed to provide financial support for the School.

The School has been organized jointly by the International Tomography Center (Novosibirsk, Russia) and by the Voevodsky Institute of Chemical Kinetics and Combustion (Novosibirsk, Russia). Conference chairs were Prof. Konstantin Ivanov (ITC) and Prof. Leonid Kulik (ICKC), Dr. Dmitri Stass (ICKC) served as the scientific secretary. Together with Dr. Maxim Yulikov (ETH Zurich, Switzerland) and Prof. P. K. Madhu (TIFR Hyderabad, India) this team was in charge of the teaching program and technical organization of the event, and aims to organize a traditional School with physical presence in Roshchino when international travelling is allowed again.

Further details can be found at the School's website: http://roshchino2020.tomo.nsc.ru.

Konstantin Ivanov
Leonid Kulik
Dmitri Stass

POSITIONS

Silicon Quantum Technology EPR Technician Position

The Silicon Quantum Technology group (http://www.sfu.ca/physics/siliconquantum), based at Simon Fraser University's campus in Burnaby, Canada, has an immediate opening for an EPR Technician. This is a full-time, grant-funded position for an initial contract period of one year, renewable for an additional three years, at a starting salary rate of $69K CAD p.a. plus benefits.

The primary responsibilities of the successful candidate will be to design, purchase components and test equipment for, assemble, build, code, and maintain a combination EPR/ENDOR spectrometer to be used by the Silicon Quantum Technology group to perform their research. This spectrometer will be used to apply advanced CW and pulse sequences to samples often held at cryogenic temperatures and in concert with external equipment such as pulsed and/or CW optical and electrical signals. The data resulting from these experiments may be in the form of traditional EPR measurements or other signals such as electrical or optical measurements. Home-built or customized open-source software will be constructed to coordinate the delivery of these sequences and capture the resulting data, and this software will have an intuitive user interface, with live and saved data display options, and it will organize data for later retrieval.

The ideal candidate will have a Bachelor's degree in Physics or Engineering with courses or formal training in microwave (MW), radio-frequency (RF) and DC electronics/electrical technology, computing systems and programming, mechanical systems, and the use of machine tools and related equipment and a minimum of 4 years related work experience. Full details are available at: https://www.sfu.ca/physics/research/groups/silicon-quantum-technology/research-EPR-technician-job.html.

All qualified candidates are encouraged to apply; however, Canadian citizens and permanent residents will be given priority.

Contact: Dr. Stephanie Simmons, s.simmons@sfu.ca, 778-782-3673

Bruker EPR Opening

The EPR Division of Bruker BioSpin has two openings for the Billerica, MA, USA office.

Application Scientist

– Ph.D. in the following areas is a prerequisite for this position: Chemistry, Biochemistry, Physics, Molecular Biology.
– Postdoctoral experience is desirable.
– U.S. Citizenship or U.S. Permanent Resident status required.

The official posting is at:
https://englishcareers-bruker.icims.com/jobs/7800/epr-application-scientist---bruker-biospin-epr-team/job?hub=12&mobile=false&width=940&height=500&bga=true&needsRedirect=false&jan1offset=-300&jun1offset=-240

Field Service Engineer

– Minimum 3 years Life Sciences Field Service work experience diagnosing and repairing complex mechanical, electromechanical and/or electronic equipment required with demonstrated mathematical abilities.
– Bachelor Degree desirable in Electrical Engineering, Electronics, Chemistry related fields.
– U.S. Citizenship or U.S. Permanent Resident status required.

The official posting is at:
https://englishcareers-bruker.icims.com/jobs/7795/field-service-engineer---bruker-biospin-epr/job?hub=12

PhD position: DNP/MAS NMR using photo-excited triplet states

The research group of Dr. Guinevere Mathies in the Department of Chemistry at the University of Konstanz is looking for an enthusiastic PhD student to join our international team. He or she will investigate if and how the high polarization generated in the photo-excited triplet states of organic molecules can be used for Dynamic Nuclear Polarization (DNP). This project is part of a larger effort in our group to develop new forms of DNP to enhance the sensitivity of high-resolution magic-angle spinning (MAS) NMR.

The candidate we look for has a MSc degree in Physics, Chemistry or a related field and research experience in EPR spectroscopy is very welcome. He or she is highly motivated, driven by curiosity, and can work independently as well as in a team.

The PhD position is planned for 3 years with the possibility of extension and a salary according to the German TVL E13 67% scale. It is available immediately and applications will be considered until the position is filled. To apply, send a cover letter and a CV to Dr. Guinevere Mathies at guinevere.mathies@uni-konstanz.de.

For more information, visit our website: https://www.chemie.uni-konstanz.de/mathies

EQUIPMENT

Walker Scientific Electromagnet

I have a Walker Scientific HF-12H Electromagnet available for donation. The magnet has 12" diameter flat pole faces and a 4.5 inch gap. It has a standard H-frame style yoke that rests on a cradle that positions the yoke at a 45 degree angle typical for EPR. The magnet is 30 years old and was always used with a closed, deionized water cooling system.

Contact: John McCracken
mccracke@msu.edu,
517 151-1159

For Sale: A Bruker ELEXSYS E500 housed at Vanderbilt University. The instrument purchased in 2000 is equipped with a SuperX bridge. The console was upgraded with a new field controller and MBC boards. The instrument is being sold as a unit including the magnet, bridge and console.

For details, please contact Hassane Mchaourab: Hassane.mchaourab@vanderbilt.edu.

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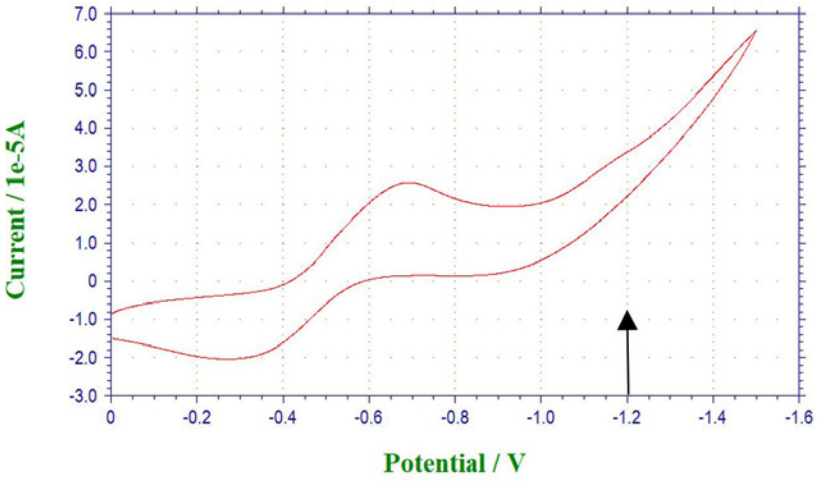

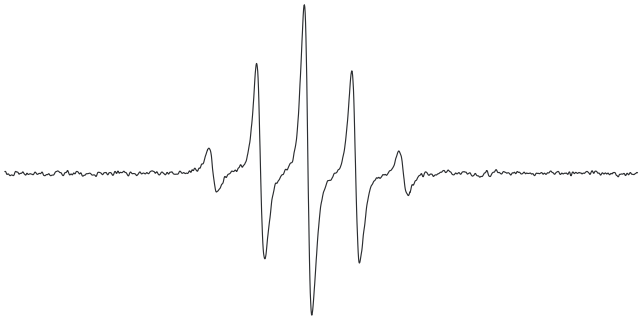

Reduction of Benzoquinone
Left, cyclical voltammetry curve.
Right, EPR spectrum at -1.2 V of the resultant benzosemiquinone radical anion.

Electrochemistry with a Benchtop EPR spectrometer. Identify species and explore reaction mechanisms in redox reactions

- In situ Cyclic Voltammetry
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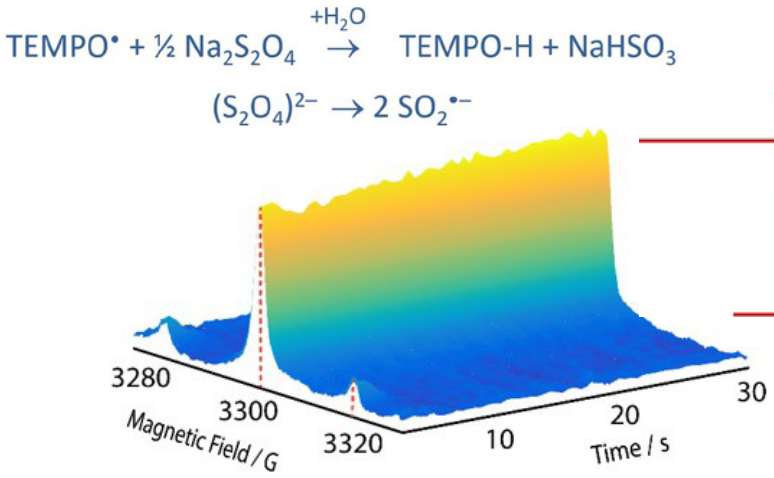

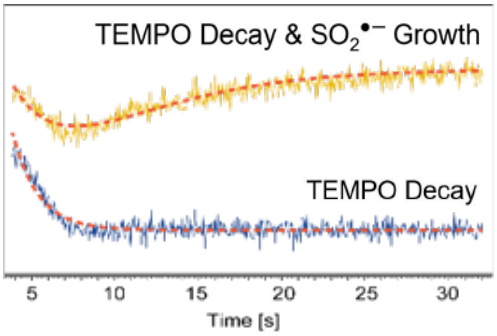

TEMPO reduction by dithionite.
Left, full spectrum during reaction.
Right, kinetic curves at center and high field positions.
Time resolution of 50 ms over 32 s.

Full 2D spectrum kinetics in the time of a single 1D CW-EPR sweep.
No need to remake solutions: EPR spectrum and kinetics in one go.

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