The 58th Annual International Meeting

of the

ESR Spectroscopy Group

of the

Royal Society of Chemistry

University College London

1st – 5th June 2025

ROYAL SOCIETY OF CHEMISTRY | ESR SPECTROSCOPY GROUP

UCL

Contents

Welcome

It is our pleasure to welcome you to University College London for the 58th International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry. We have approximately 120 delegates registered for the conference with broad national and international representation, reflecting the thriving community centred upon electron spin resonance spectroscopy. We hope you enjoy the conference with its exciting programme of talks, posters and opportunities to network, socialise and enjoy London.

We are delighted to celebrate the 40th Bruker Prize awarded to Stephen Hill for his seminal contributions to EPR in terms of both world-leading instrument design and imaginative application of high field EPR to the study of low dimensional systems. Furthermore, we are thrilled to applaud Yujie Zhao, the recipient of the 11th Bruker Thesis Prize for her investigation of DNP and ENDOR using high frequency EPR. We continue to be grateful to Bruker for their generous support of this conference and using it as a platform for highlighting these highly competitive awards.

The continuously close relationship between the RSC ESR interest group and the International EPR Society (IES) allows the IES Annual General Meeting to be held during the conference on Tuesday 3rd June and we are also pleased to host the IES John Weil Young Investigator Award talk by Nino Wili. The Committee and IES are pleased to announce that two poster prizes sponsored by the IES will be awarded to the best poster presentations by young researchers. All posters presented by young researchers at the conference will automatically be considered for these prizes. Prizes will include one year of free IES membership.

We extend our heartfelt thanks to JEOL for their steadfast support and sponsorship of the prize for best talk from an early career researcher. Thanks also to our sponsors: Bruker, ICEoxford, CIQTEK, High Q Technologies, JEOL, AMP (Amplify my Probe), SCIMED, QBLOX, Cryogenic and IES. Please ensure to engage with their representatives during the conference to discuss ESR spectroscopy and learn about their products.

Our personal thanks go to the RSC ESR Spectroscopy Group who have provided invaluable input into planning of this conference. We particularly wish to thank Christiane Timmel for her tireless efforts and her sterling work as the Chair of the Committee these past years. We would also like to thank the incoming Chair Emma Richards, Christopher Wedge and Will Myers for their valued contributions.

We would finally like to thank our team of assistants and you the delegates for participating in ESR 2025 London – we hope you have a wonderful time!

With our very best wishes,

Jonathan Breeze, John Morton & Sarah Smerald

University College London, 2025

Information

We look forward to welcoming you to London in June for the 58th International Meeting of the RSC ESR Group. The main conference will take place over 3.5 days in Mary Ward House, in the heart of Bloomsbury in Central London, with a banquet dinner at Ironmongers' Hall on the Wednesday evening preceded by an optional walk along the River Thames.

Following an optional evening social event on Sunday 1st June from 6.00pm onwards, the main conference will run from 9.00am on Monday 2nd June through to lunchtime on Thursday 5th June.

Venue

The conference venue, Mary Ward House, is ideally located in Central London, Bloomsbury (https://www.marywardhouse.com/location):

Mary Ward House,
7 Tavistock Place, London,
England,
WC1H 9SN,
United Kingdom
02073879681
info@marywardhouse.com

Travel Information

National rail (UK) or Eurostar (International).

The conference venue is within walking distance of Euston, St Pancras and King's Cross mainline stations (all within 15 minutes). St Pancras station is the London Eurostar terminal with direct high speed rail connections to Paris (2hrs 15 mins) and Brussels (1hr 50 mins), with onward connections to many European destinations. We encourage use of trains to travel to London, where possible.

Air

London is served by five main airports (London City, Heathrow, Gatwick, Luton and Stansted), listed in approximate order of convenience for reaching the conference venue. Use directions below for reaching the conference venue in the Bloomsbury area of London. We recommend using rail and tube services to travel to/from airports and avoiding taxis.

London Underground (Tube)

The closest Tube stations to Mary Ward House are **Russell Square** (Piccadilly line), **Euston Square** (Hammersmith and City, Metropolitan and Circle lines), **Euston** (Northern and Victoria lines) all within a 6-10 minute walk.

You can use most contactless bank cards to use the Tube, or buy an Oyster card. See the London Underground information and journey planner (Transport for London) for more information.

Programme

A Welcome Reception will be held at **The Marquis Cornwallis** pub from 6pm on Sunday 1st June.

Address: The Marquis Cornwallis, 31 Marchmont Street, WC1N 1AP, London
Website: https://www.themarquiscornwalliswc1.co.uk

Banquet

On the evening of Wednesday 4th June, the banquet dinner will be held at **Ironmongers' Hall**.

Address: Shaftesbury Place, off Aldersgate Street, Barbican, London EC2Y 8AA.
Google Maps link
3D view link
https://www.ironmongers.org

A reception will be held from 6:30pm until 7:45pm followed by dinner.

Monday 2nd June

8:00 – 8:45	Registration
8:50 – 9:00	**John Morton (UCL), *Welcome & Safety Information***
Session 1 (Chair: Janet Lovett)	
9:00 – 9:40 Plenary talk	**Sabine Van Doorslaer (University of Antwerp)** ***Exploiting the EPR toolbox in copper(II) chemistry***
9:40 – 10:00	Bela Bode (University of St Andrews) *Investigating protein structure and function through para-magnetic substitution of native metal ions*
10:00 – 10:20	Eleanor Clifford (Imperial College London) *Characterisation of a semiquinone radical bound in the active site of respiratory complex I by hyperfine EPR spectroscopy*
10:20 – 10:50	Tea & Coffee
10:50 – 11:10	Joshua Harbort (CNRS & Université Aix-Marseille) *EPR and HYSCORE spectroscopic characterisation of the coordination of the ferric thiolate haem cofactor in a de novo designed protein mimicking natural cyt P450 monooxygenases*
11:10 – 11:30	Dima Svistunenko (University of Essex) *EPR can follow electron hole hopping in proteins - but can we design new routes?*
11:30 – 11:50	Daniel Klose (ETH Zürich) *Progress and challenges in combining EPR & DFT for chemical insights into Ti(III)-based catalysts*
11:50 – 12:10	Joshua Wort (University of Manchester) *Conformational dynamics and asymmetry in multimodal inhibition of membrane-bound pyrophosphatases*
12:10 – 13:40	Lunch
Session 2 (Chair: Paul Jonsen)	
13:40 – 14:10 Invited talk	**Enrico Salvadori (University of Torino)** ***Native and photo-induced paramagnetic species in carbon nitride photocatalysts***
14:10 – 14:30	Mikhail Agrachev (ETH Zürich) *EPR investigation of anionic vacancies: semiconductor physics and heterogeneous catalysis*
14:30 – 14:50	Andrei Kuzhelev (Goethe University Frankfurt) *High-field dynamic nuclear polarization in liquids: Toward biomolecular applications*
14:50 – 15:10	Stergios Piligkos (University of Copenhagen) *Population transfers in a molecular 4f qudit*
15:10 – 16:30	Poster Session 1 and Tea & Coffee
16:30 – 16:50 JEOL Prize	Jack Palmer (University of Oxford) *From charge-transfer states to separated charges: organic photovoltaics probed by transient and pulse EPR*
16:50 – 17:10 JEOL Prize	Annemarie Kehl (Max Planck Institute) *Frequency and time domain ^{19}F ENDOR spectroscopy: role of nuclear dipolar couplings to determine distance distributions*
17:10 – 17:30 JEOL Prize	Hannah Eckvahl (Northwestern University) *Direct detection of the chirality induced spin selectivity effect in donor acceptor molecules*
17:30 – 18:00	Break
18:00 –	JEOL Reception

Tuesday 3rd June

Session 3 (Chair: Enrico Salvadori)	
9:00 – 9:40 Plenary talk	**Sandrine Heutz (Imperial College London)** ***Exploiting spins in molecular semiconductors - from solar cells to quantum tech***
9:40 – 10:00	Alexander Schnegg (Max Planck Institute) *Zero-field splittings in metalloarsinidene and organobismuthinidene studied by FD-FT THz-EPR*
10:00 – 10:20	Graham Smith (University of St Andrews) *Wideband techniques in HF EPR*
10:20 – 10:50	Tea & Coffee
10:50 – 11:10	Yury Kutin (TU Dortmund University) *A monosubstituted C(0) atom in its triplet state: expanding the family of carbon-centred diradicals*
11:10 – 11:30	Naitik Panjwani (Freie Universität Berlin) *Bright triplet and charge-separated singlet excitons in organic diradicals enable optical addressability of spin states*
11:30 – 11:50	Jeannine Grüne (University of Cambridge) *High-spin state dynamics and quintet-mediated emission in singlet fission systems*
11:50 – 12:10	Kaltum Abdiaziz (Max Planck Institute) *Harnessing the potential of spectroelectrochemical EPR: design and application*
12:10 – 12:40 Invited talk	**Alice Bowen (University of Manchester)** ***A tale of two light-induced EPR experiments***
12:40 – 13:30	Lunch
13:30 – 14:10	**Bruker Demo**
14:10 – 15:40	Poster Session 2 and Tea & Coffee
Bruker Thesis Prize (Chair: Jeannine Grüne)	
15:40 – 15:50	**Laudatio: Graham Smith**
15:50 – 16:20 **Bruker Thesis Prize**	**Yujie Zhao** **Massachusetts Institute of Technology** ***Methodology development of high sensitivity pulsed EPR and DNP***
IES Young Investigator Award	
16:20 – 16:25	**Laudatio: Marina Bennati**
16:25 – 16:55 **IES Young Investigator**	**Nino Wili** **Aarhus University** ***Improved multi-pulse sequences for hyperfine spectroscopy and dynamic nuclear polarisation***
16:55 – 17:05	Break
17:05 – 18:05	IES General Assembly
18:05 –	Free Evening

Wednesday 4th June

Session 4 (Chair: Christopher Kay)	
9:00 – 9:40 **Plenary talk**	**Emmanuel Flurin (CEA Saclay)** ***Single spin magnetic resonance by microwave photon counting***
9:40 – 10:00	Aharon Blank (Technion - Israel Institute of Technology) *Solid-state maser with microwatt output power at moderate cryogenic temperatures*
10:00 – 10:20	Siddharth Dhomkar (Indian Institute of Technology Madras) *Utilizing optimal magnetic field configurations for mitigating decoherence in optical spin defects*
10:20 – 10:50	Tea & Coffee
10:50 – 11:10	Fabio Donati (IBS Center for Quantum Nanoscience, Ewha Womans University) *Surface-ensemble electron spin resonance of ultra-thin YPc_2 films as a potential molecular spin qubit architecture*
11:10 – 11:30	Patrick Hogan (University College London) *Hyperpolarizing ^{209}Bi:Si nuclear spins using superconducting microresonators*
11:30 – 11:50	Mantas Šimėnas (Vilnius University) *Superconducting spiral microresonators enable versatile high sensitivity EPR*
11:50 – 12:10	Hugo Karas (ETH Zürich) *autoDEER – fully automated DEER spectroscopy*
12:10 – 13:40	Lunch
Session 5 (Chair: Emma Richards)	
14:00 – 14:30 **Invited talk**	**Helena Knowles (University of Cambridge)** ***Electron spin resonance at the nanometre scale using diamond quantum sensors***
14:30 – 14:50	Ravi Acharya (University of Melbourne) *Low-field magnetic clock transition of near-surface ^{75}As spins in silicon via electrically detected magnetic resonance*
14:50 – 15:10	Philipp Thielert (University of Freiburg) *Spin mixing in supramolecular light-induced multi-spin systems*
15:10 – 15:40	Tea & Coffee
15:40 – 15:50	**Laudatio: Stephen Blundell**
15:50 – 16:40 **Bruker Prize**	**Stephen Hill** **Florida State University and National High Magnetic Field Laboratory** ***From molecular magnetic clusters to spin qubits: a high-field EPR spectroscopist's retrospective***
16:40 – 17:00	Break
17:00 – 19:00	London Riverwalk
19:00 –	Bruker Banquet

Thursday 5th June

Session 6 (Chair: Christiane Timmel)	
9:30 – 10:00 Invited	**Elisabetta Mileo (CNRS & Université Aix-Marseille)** ***In-cell EPR: A combined approach using nitroxide radicals, SDSL and EPR to probe protein behaviour within cells***
10:00 – 10:20 Contributed	Alexey Bogdanov (Weizmann Institute of Science) *F ENDOR as a means to determine the orientation of zero-field splitting tensor in Gd(III) chelates*
10:20 – 10:40 Contributed	Alistair Fielding (Liverpool John Moores University) *Rotamer library analysis and investigations of the properties of the bromoacrylaldehyde spin label*
10:40 – 11:10	Tea & Coffee
11:10 – 11:30 Contributed	Gabriela Ionita (Ilie Murgulescu Institute of Physical Chemistry) *Host-guest complexes of various nitroxides as potential contrast agents for OMRI applications*
11:30 – 11:50 Contributed	Janet Lovett (University of St Andrews) *Citius, Altius, Fortius: New spirocyclic nitroxide spin labels*
11:50 – 12:30 Plenary	**Ilya Kuprov (Weizmann Institute of Science)** ***Instrumental effects in optimal control pulse design***
12:30 – 12:45	Closing Remarks and announcement of RSC ESR 2026
12:45	Conference Ends

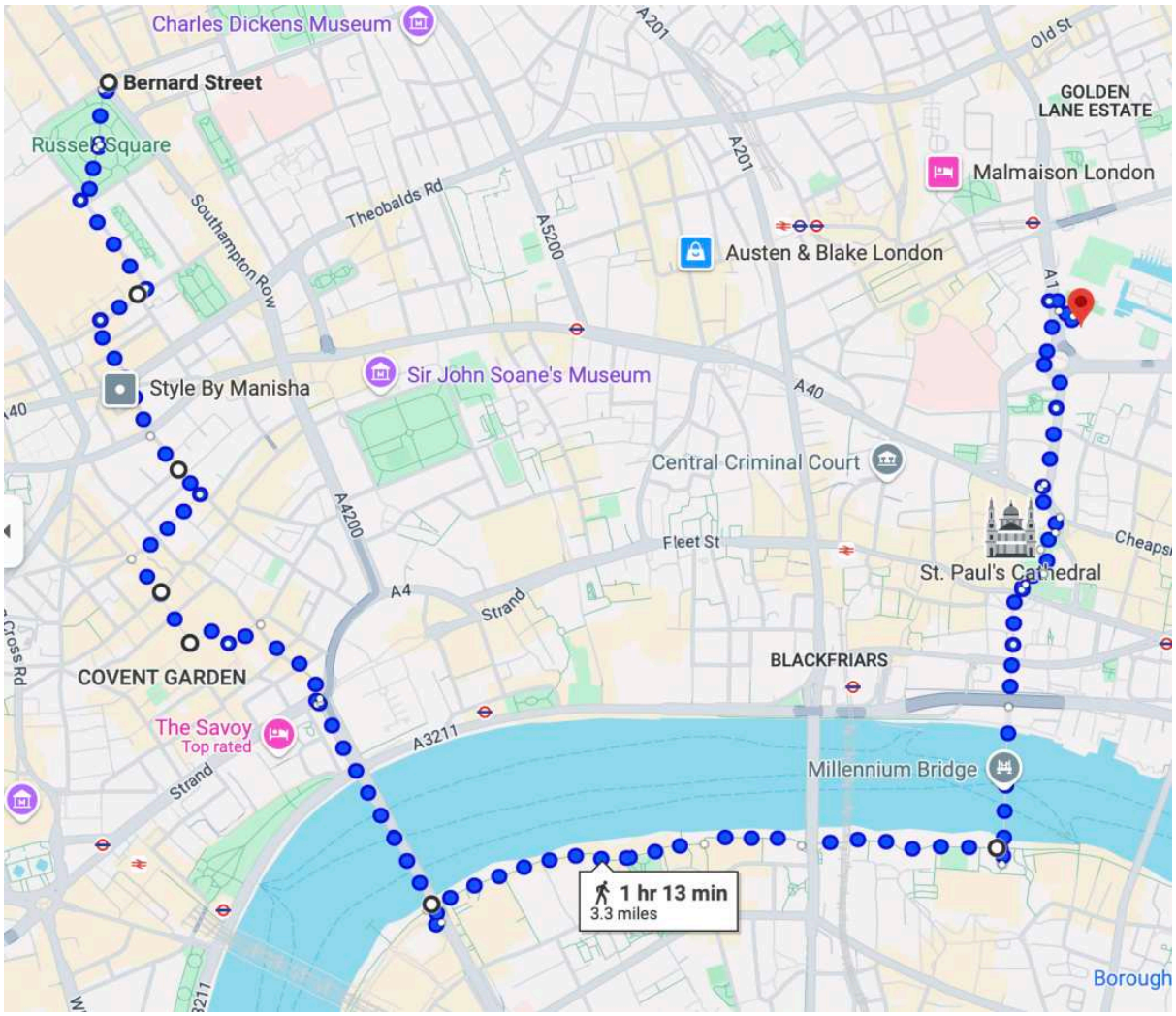
London Riverwalk to Ironmongers' Hall
5pm Wednesday 4th June

We have four different routes available with varied distances of 1.7, 3.3, 3.8 (walking) and 6.3 miles (cycling). There will be guides to lead the way.

Please sign up for a particular route (or none!) with Registration during the week.

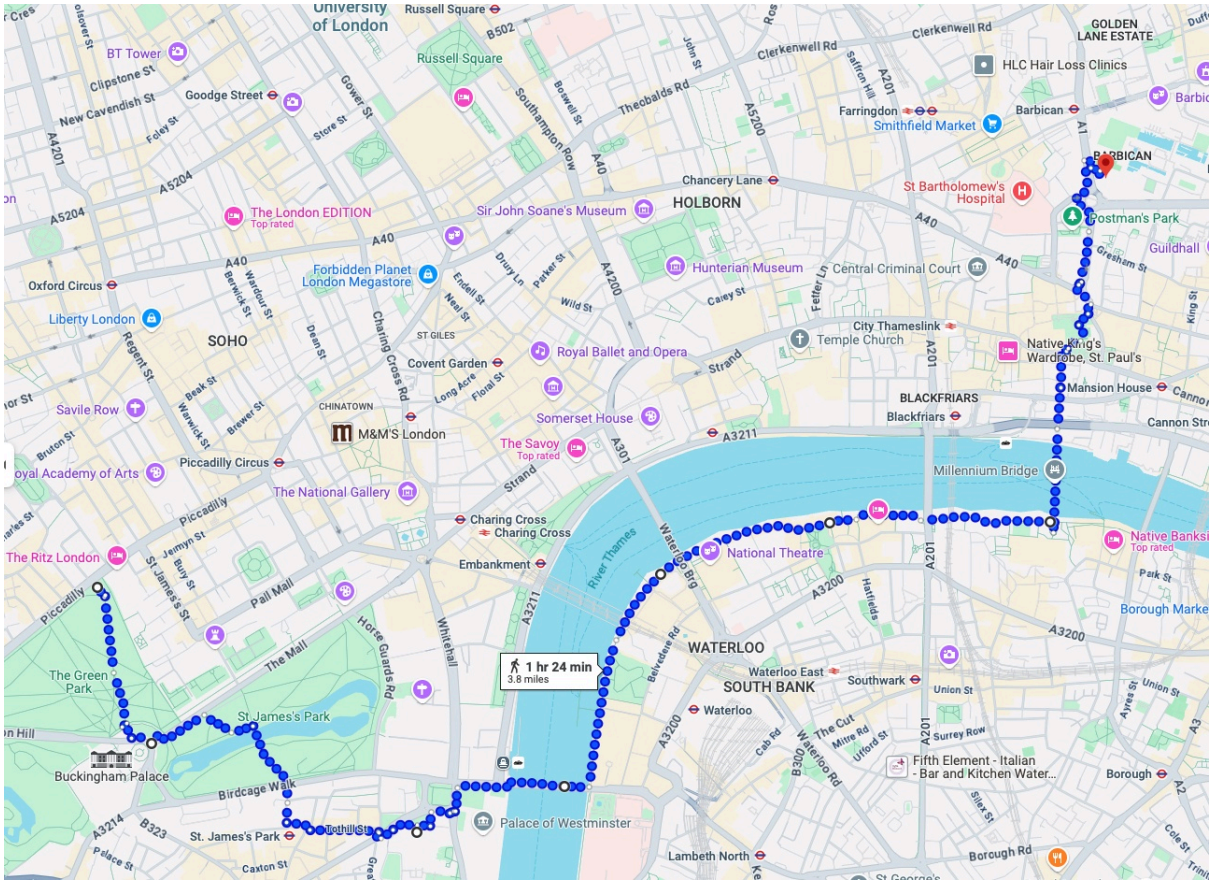
Route 1: Leave 5pm from Venue. 3.3 mile walk (1hr 20 mins)

- British Museum
- Covent Garden
- South bank
- Tate Modern
- Millenium Bridge
- St Paul's Cathedral



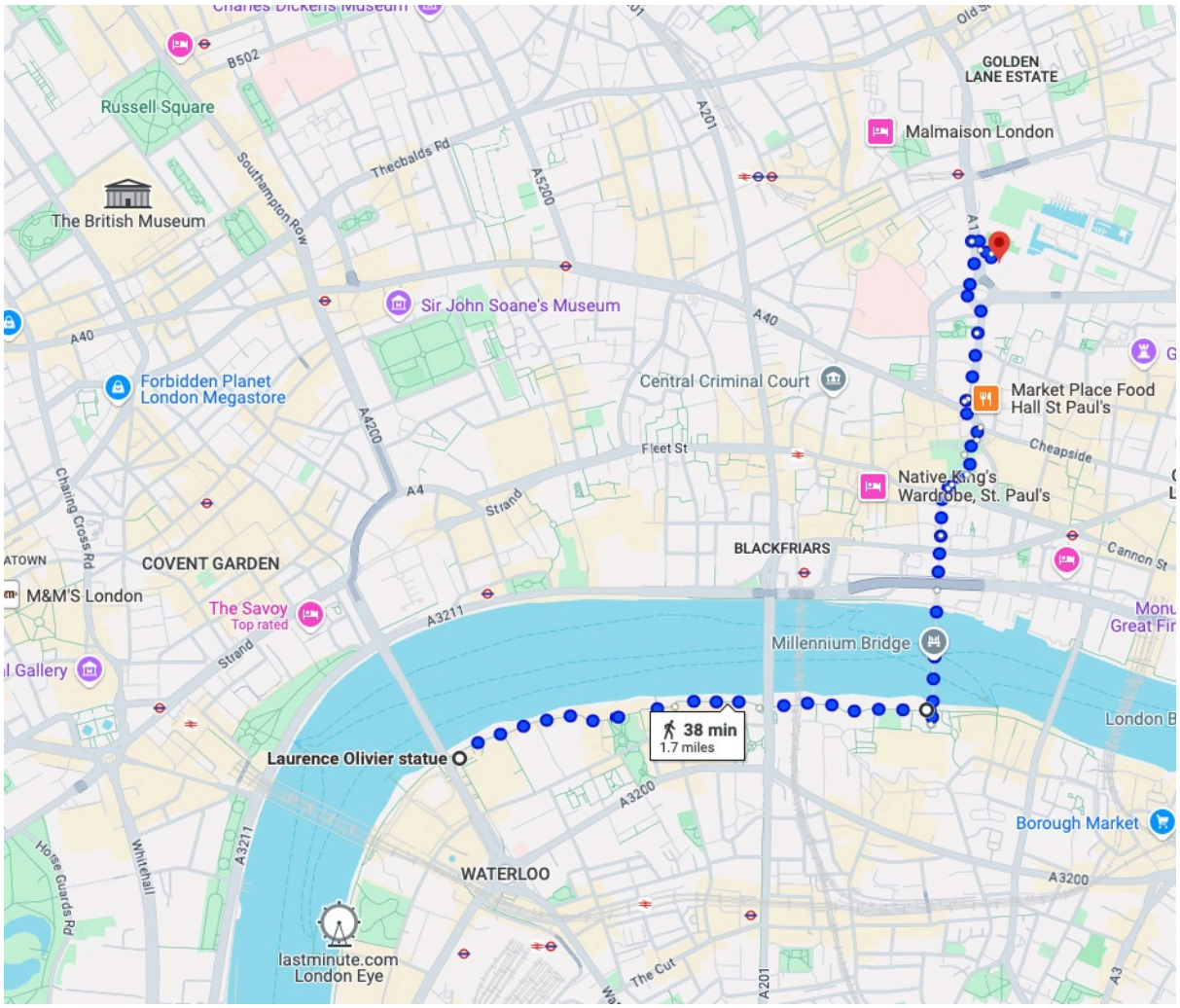
Route 2: Leave 5pm from **Green Park Tube** station (or 4:45pm from Russel Square Tube station). **3.8 mile walk (1hr 30mins)**

- Buckingham Palance
- Westminster Abbey
- Big Ben
- South bank
- Tate Modern
- Millenium Bridge
- St Paul's Cathedral



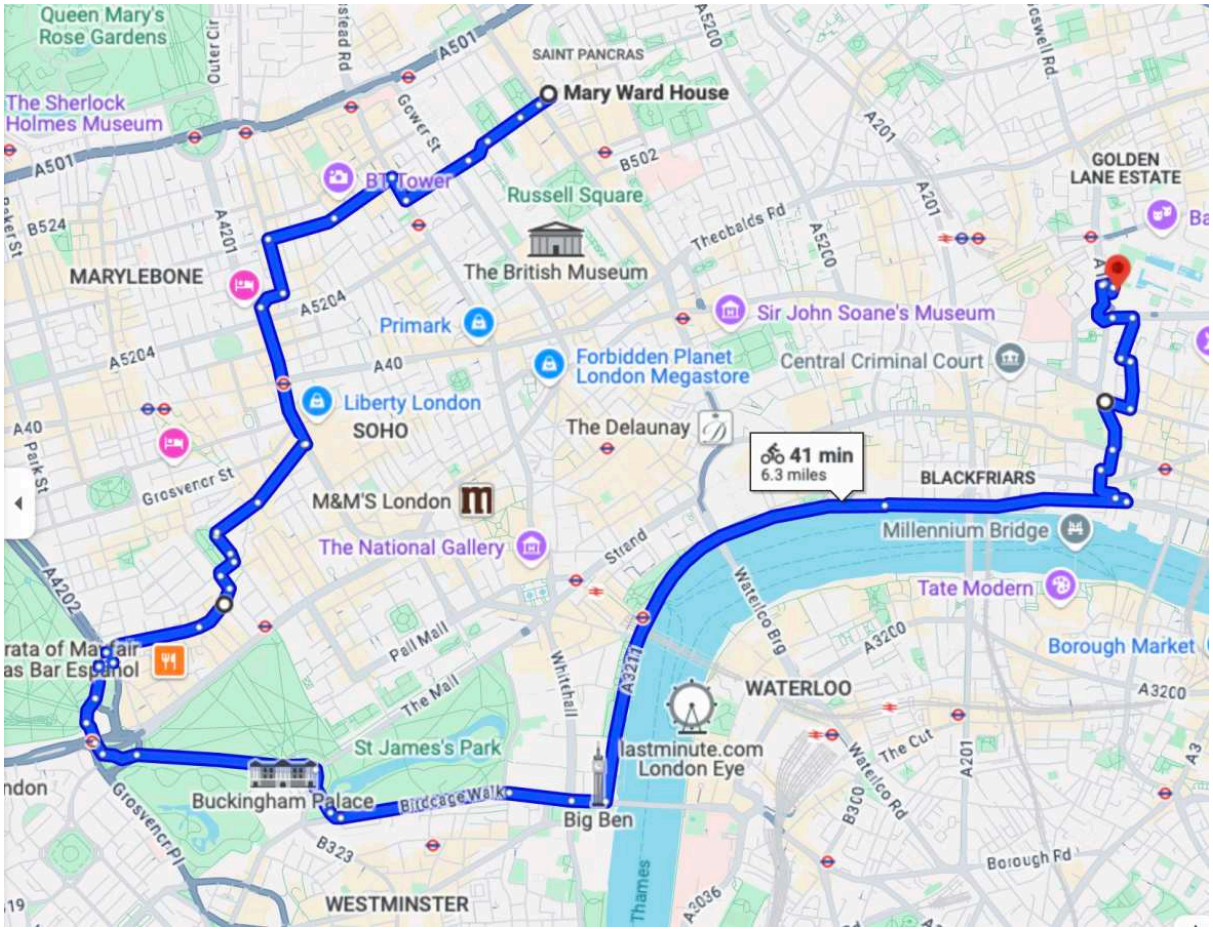
Route 3: Leave 6pm from **National Theatre / Laurence Olivier Statue** (Can get 25 min bus from venue to Waterloo Bridge). 1.7 mile walk (45 mins)

- South bank
- Tate Modern
- Millenium Bridge
- St Paul's Cathedral



Route 4: Cycle Tour (6.3 miles). Leave 5pm from **Mary Ward House**

- Oxford Circus
- Mayfair
- Buckingham Palance
- Westminster Abbey
- Big Ben
- Embankment
- St Paul's Cathedral



Bruker Prize Lecture 2025

Stephen Hill

Since 1986 Bruker BioSpin has generously sponsored an annual lectureship and prize, given to a scientist who has made a major contribution to the application of ESR spectroscopy in chemical or biological systems. The RSC ESR Spectroscopy Group and Bruker are excited to announce the Bruker lecturer 2025 **Professor Stephen Hill** for,

> *his seminal contributions to EPR in terms of both world-leading and unique instrument design as well imaginative and expert application of high field EPR to the study of low dimensional systems. His work has opened up new avenues for EPR driven developments including in, but not limited to, the fields of quantum information science and the study of polymetallic transition metal complexes. Crucially, as Director of the Electron Magnetic Resonance user program at the NHMFL he has supported and fostered the international and national EPR communities with unique scientific expertise and admirable dedication.*

The 2025 Bruker lecture is the 40th Anniversary of this prestigious prize, and we are excited to celebrate this milestone and Stephen's achievement at the London conference in June 2025. The list of winners of the previous 39 prizes Bruker Prize is available here. We are grateful to Bruker for their longstanding support of this prize.

From Molecular Magnetic Clusters to Spin Qubits: a High-Field EPR Spectroscopist's Retrospective

Stephen Hill[1]

[1] Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee FL 32310, USA

This presentation will be loosely based on a recent article written for the American Physical Society magazine, Physics Today [1], focusing on my own journey, made possible thanks to so many phenomenal collaborations over the years. It is a journey that began with an accidental encounter with the Mn_{12}-acetate molecular cluster, made famous for the beautiful quantized steps observed in its low-temperature magnetization hysteresis curves. Those results clearly demonstrated quantum tunneling of a magnetic moment through an anisotropy energy barrier for the first time, opening up a spectacular playground for high-field EPR spectroscopists. As the field has evolved from studies of large transition metal clusters to molecules containing single lanthanide ions, interest has also grown from an initial focus on classical magnetic data storage to recent emphasis on quantum information science. I will review the critical importance of multi-/high-frequency EPR throughout this evolution, beginning with the characterization of interactions responsible for magnetic quantum tunneling and, more recently, the identification of so-called spin clock transitions – optimal qubit operating points that protect against spin-spin decoherence. Of course, this story could never be told without highlighting the contributions of so many outstanding mentors, colleagues and collaborators, which I shall do throughout the presentation.

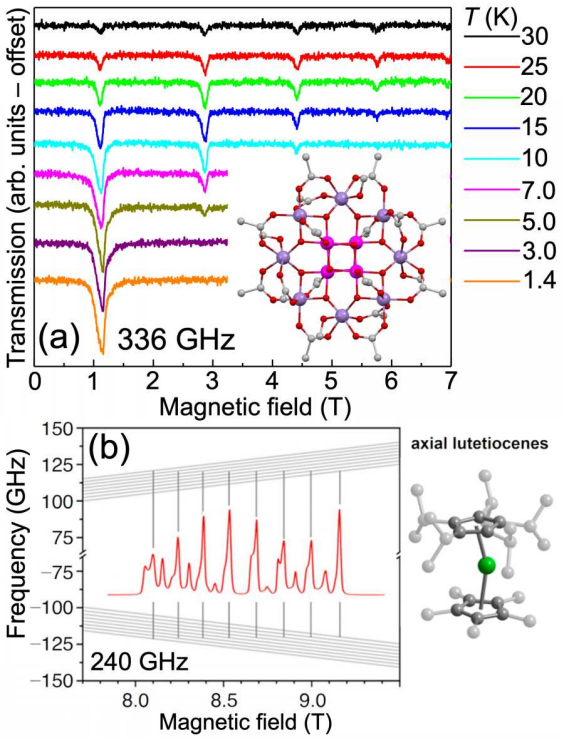


Fig. 1: (a) Temperature dependent high-field EPR spectra of a $[Mn_{12}O_{12}(O_2CCH_2Bu^t)_{16}(MeOH)_4]\cdot MeOH$ (inset: Mn^{IV} – pink, Mn^{III} – purple, O – red, C – gray) single crystal [2]. (b) Hyperfine spectrum and energy level diagram of the $S = ½$, $I = {}^7/_2$ $Lu^{II}(Cp^{Me5})(Cp^{iPr5})$ (Cp^{Me5} = pentamethylcyclopentadienyl; Cp^{iPr5} = penta-isopropylcyclopentadienyl) molecular spin qubit (shown right: Lu^{II} – green, C – gray) [3].

[1] *Making Qubits from Magnetic Molecules*, Stephen Hill, Physics Today **78**, 38 – 45 (2025). https://doi.org/10.1063/pt.keiz.kcmn
[2] Lampropoulos et al., Inorg. Chem. **52**, 258 – 272 (2012).
[3] Ngo et al., J. Am. Chem. Soc. **147**, 13799 – 13807 (2025).

Bruker Thesis Prize 2025

Yujie Zhao

The ESR Group of the Royal Society of Chemistry and Bruker Corporation are pleased to announce the winner of the 11th Bruker ESR Thesis Prize is Dr Yujie Zhao. As winner of the 2025 competition, Dr Zhao has accepted an invitation to give a prize lecture at the 58th Annual International Meeting of the RSC ESR spectroscopy group, in London, 1st to 5th June 2025.

Dr Yujie Zhao completed her doctoral thesis, titled "Methodology development of high sensitivity pulsed EPR and DNP", in the mm-Wave and EPR group at the University of St Andrews, Scotland, under the supervision of Prof. Graham Smith. Our international judging panel were impressed with the breadth of the thesis, spanning both EPR and DNP investigations. One reviewer described the work as:

"*an excellent example of a thorough investigation of DNP and ENDOR using high frequency EPR with timely and relevant insights and conclusions for both EPR and solid-state DNP NMR from the design and building of hardware, experimental implementation, theory, simulation and experiment and application to a contemporary research area*"

Meanwhile another expert external reviewer praised the significant hardware developments reported in the thesis, which "*pushed the boundary of pulsed W-band DNP through extraordinary instrumentation capabilities*". We look forward to hearing about this work in the thesis prize lecture which will take place on Tuesday 3rd June 2025.

Methodology development of high sensitivity pulsed EPR and DNP

Yujie Zhao,[1*] Hassane El Mkami,[1] Robert Hunter,[1] Graham Smith[1]

[1] Millimetre wave and EPR group, School of physics and astronomy, University of St Andrews, St Andrews, United Kingdom, KY16 9SS;

*Current address: Francis Bitter Laboratory, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, United States, 02139

Dynamic nuclear polarisation (DNP) is a process that transfers electron spin polarisation to nuclei and is a technique that has been widely used to improve nuclear magnetic resonance (NMR) sensitivity. This thesis presents the implementation of a DNP extension to a home-built high power pulsed electron paramagnetic resonance (EPR) spectrometer, HiPER, integrated with an arbitrary waveform generator (AWG), operating at 94 GHz. It describes the use of high-peak power inverting chirped pulses to increase the polarisation gradient of dipolar-coupled electrons, where static cross-effect DNP enhancements of 340 are achieved within 3 seconds at 65 K with a mixture of 4-amino TEMPO and DNP juice. Several other nitroxide radical polarising agents are also investigated and systematic study into the DNP temperature dependence for different polarising agents reveals the impact of spectral diffusion and the molecular structure of polarising agents.

In addition, for the first time at 94 GHz, a comparative study is made of different coherent pulsed solid-effect DNP schemes including XiX, TPPM, and the adiabatic solid-effect. An ENDOR upgrade to the DNP/EPR spectrometer is also described, and preliminary room-temperature ^{1}H ENDOR and low-temperature ^{19}F ENDOR experiments presented, where a combined approach involving shaped pulse excitation and data processing at an intermediate frequency in down-conversion for DC suppression yields a threefold enhancement in SNR. Finally, a brief summary to other projects on EPR probe design, magnet shimming, transition metal DNP and DNP characterisation for lithium dendrites is provided.

[1] Methodology development of high sensitivity pulsed EPR and DNP. Zhao, Y. (Author). 10 Jun 2024. *Student thesis: Doctoral Thesis (PhD)*
[2] Zhao, Y., El Mkami, H., Hunter, R.I. *et al.* Large cross-effect dynamic nuclear polarisation enhancements with kilowatt inverting chirped pulses at 94 GHz. *Commun Chem* **6**, 171 (2023). https://doi.org/10.1038/s42004-023-00963-w

International EPR Society

John Weil
Young Investigator Award 2025

Nino Wili

The 2025 John-Weil Young Investigator Award of the International EPR (ESR) Society is awarded to Dr. Nino Wili for his contributions to theory and instrumentation in the field of EPR. In particular, the IEPRS recognizes his studies that seamlessly integrate advanced concepts in pulsed EPR and in dynamic nuclear polarization.

These studies have provided new insight into spin dynamics in systems where multiple nuclear spins are hyperfine-coupled to an electron spin. Further, they have cross-fertilized the field of EPR spectroscopy with modern concepts from the field of solid-state NMR. By demonstrating reverse polarization transfer from nuclear to electron spins, Dr. Wili has opened a new field of research.

Improved Multi-Pulse Sequences for Hyperfine Spectroscopy and Dynamic Nuclear Polarisation

Nino Wili,[1] Anders B. Nielsen,[1] José P. Carvalho,[1] David L. Goodwin,[1] Niels Chr. Nielsen,[1]

[1] Interdisciplinary Nanoscience Center (iNANO) and Department of Chemistry, Aarhus University, Gustav Wieds Vej 14, DK-8000 Aarhus C, Denmark

Manipulation of electron-nuclear spin systems in pulse EPR is typically conducted with a small number of pulses. The only widespread multi-pulse sequence is CPMG, which is typically used as a dynamical decoupling sequence. In contrast, in NMR, especially in Magic-Angle-Spinning (MAS) solid-state NMR, multi-pulse sequences with repeating building blocks are ubiquitous, as they allow tailoring of the effective Hamiltonian.
In pulse EPR, pulse sequences are typically analysed with the product-operator formalism. Due to pseudosecular hyperfine couplings, this is already quite complex even for a Hahn echo. While the literature contains some heroic efforts to analyse *e.g.* 6-pulse HYSCORE experiments [1], the resulting formulas hardly provide any intuitive insight.

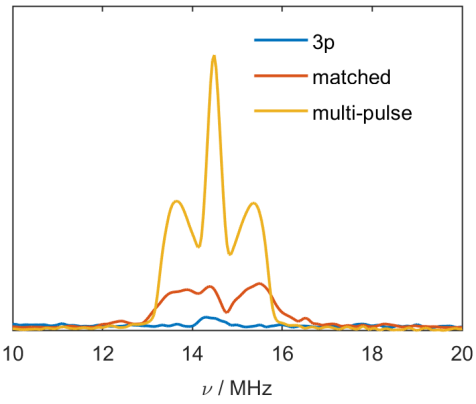


Figure 1: Improved ESEEM spectroscopy by employing multi-pulse sequences compared to the usual 3-pulse or matched ESEEM sequences. The peaks stem from weakly coupled protons in Cu(II)-TPP in a fully deuterated matrix.

In this talk, I will present some recent efforts in developing multi-pulse sequences for EPR, both theoretically and experimentally. I will present a theoretical framework that offers an intuitive understanding of these sequences and at the same time provides links to pulsed Dynamic Nuclear Polarisation (DNP) [2], dipolar recoupling in solid-state NMR, and the excitation of long-lived singlet states in nearly equivalent nuclear spin pairs [3]. Experimental results for improved ESEEM sequences (see Figure 1), as well as pulsed DNP will be shown. The latter will include some peculiar “time-reversal” experiments [4]. Experiments were conducted on a home-built spectrometer based on a fast arbitrary waveform generator with home-written software that allows easy and flexible implementation of new ideas.

[1] B. Kasumaj and S. Stoll, 5- and 6-pulse electron spin echo envelope modulation (ESEEM) of multi-nuclear spin systems, J. Magn. Reson. **190**, 233 (2008).
[2] N. Wili, A. B. Nielsen, L. A. Völker, L. Schreder, N. Chr. Nielsen, G. Jeschke, and K. O. Tan, Designing broadband pulsed dynamic nuclear polarization sequences in static solids, Sci. Adv. **8**, eabq0536 (2022).
[3] M. Sabba, N. Wili, C. Bengs, J. W. Whipham, L. J. Brown, and M. H. Levitt, Symmetry-based singlet–triplet excitation in solution nuclear magnetic resonance, J. Chem. Phys. **157**, 134302 (2022).
[4] N. Wili, A. B. Nielsen, J. P. Carvalho, and N. Chr. Nielsen, Observation of dynamic nuclear polarization echoes, Sci. Adv. **10**, eadr2420 (2024).

The JEOL Student Lecture Prize

The JEOL Student Lecture Competition began at the ESR Group Meeting at Lancaster University in 1997. In subsequent years the lectures have gained huge popularity and prestige.

This year the JEOL Student Lecture Prize session will take place on Monday 2nd June from 16:30 until 17:30.

This year's speakers are:

Jack Palmer (University of Oxford)
From charge-transfer states to separated charges: organic photovoltaics probed by transient and pulse EPR

Annemarie Kehl (Max Planck Institute)
Frequency and time domain 19F ENDOR spectroscopy: role of nuclear dipolar couplings to determine distance distributions

Hannah Eckvahl (Northwestern University)
Direct detection of the chirality induced spin selectivity effect in donor acceptor molecules

The previous 21 winners of the prize were:
Jörg Fischer, Sebastian Gorgon, Fabian Hecker, Nino Wili, Gabriel Moise, Frauke Breitgoff, Leah Weiss, Jason Sidabras, Michael Lerch, Andrin Doll, Daniel Klose, Christopher Hartland, Alice Bowen, Petra Lueders, Hans Moons, Angelika Boer, Aleksei Volkov, Sharon Ruthstein, Janet Lovett, Malika Bouterfas, Dariush Hinderberger, Stefan Stoll, and Anna Ferretti.

Committee of the ESR Spectroscopy Group of the Royal Society of Chemistry

Chair: Dr Emma Richards (University of Cardiff)

Secretary: Dr Janet Lovett (University of St. Andrews)

Treasurer: Dr Paul Jonsen (Talavera Science)

Web Master: Dr Will Myers (University of Oxford)

International Representative: Prof Marilena Di Valentin (University of Padova)

Industry Representative: Dr Alex Shread (Bruker UK Ltd)

Committee Member: Prof Enrico Salvadori (University of Turin)

Committee Member: Dr Dimitri Svistunenko (University of Essex)

Committee Member: Prof Christopher Kay (Universität des Saarlandes)

Committee Member: Dr Jeremy Lea (QUAD Systems AG)

Committee Member: Mr Adam Brookfield (University of Manchester)

Early Career Representative: Dr Jeannine Grüne (University of Cambridge)

ex-officio: Prof Christiane Timmel (University of Oxford)

RSC Networks Officer: Dr Fiona McMillan (RSC)

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Bronze sponsors

JEOL Solutions for Innovation

Amplify my Probe ltd

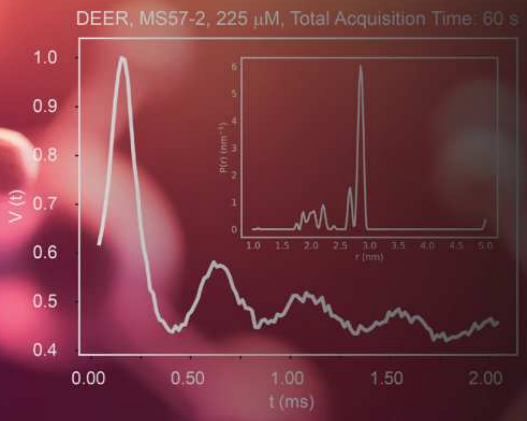
SciMED Global Brands, Local Support

QBLOX

International EPR (ESR) Society IES

EPR

Compact-Q DEER Spectrometer



Pulse Q-Band EPR Spectrometer Optimal for Pulsed Dipolar Spectroscopy (PELDOR/DEER)

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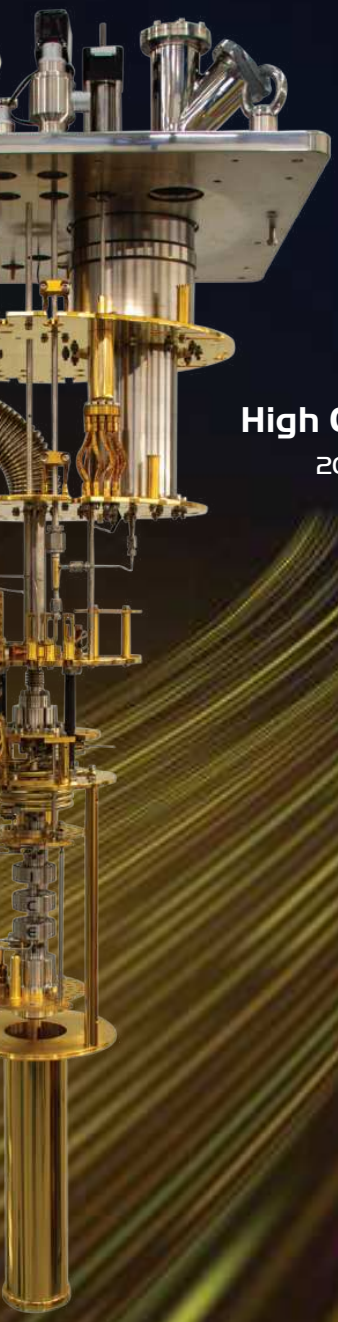

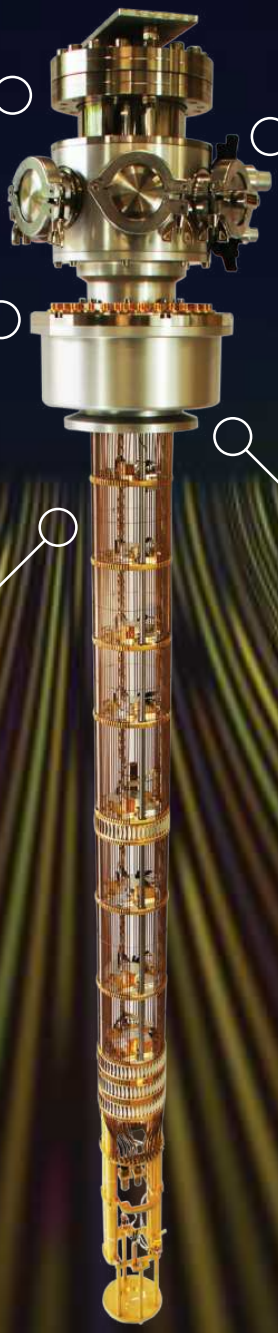

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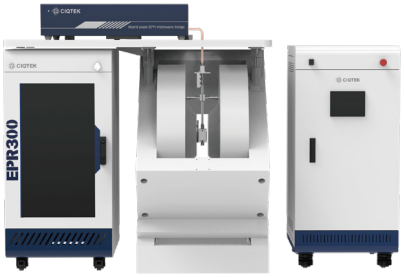

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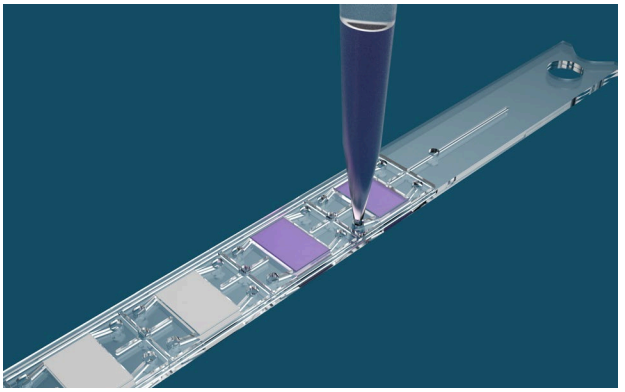

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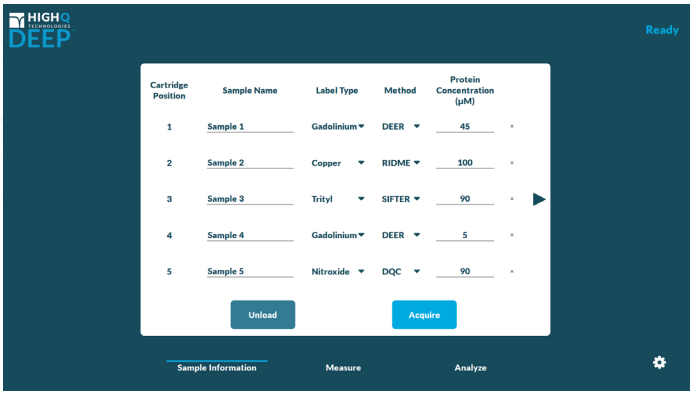

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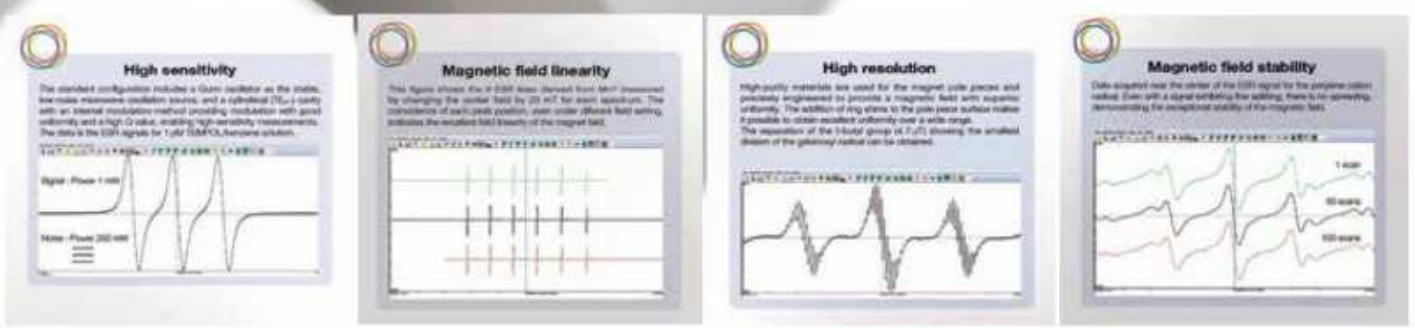

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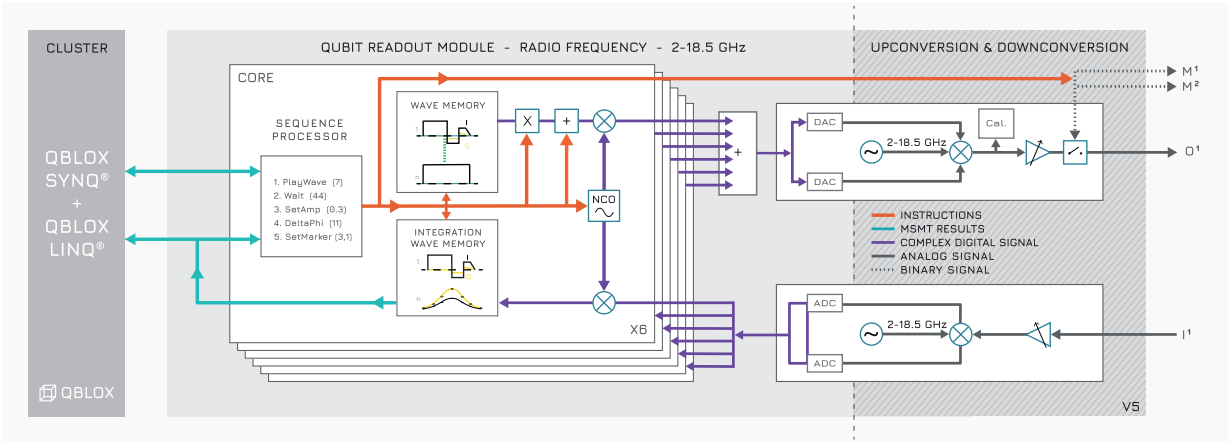

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Phase noise (@3 GHz, 10 kHz offset)	-115 dBc/Hz

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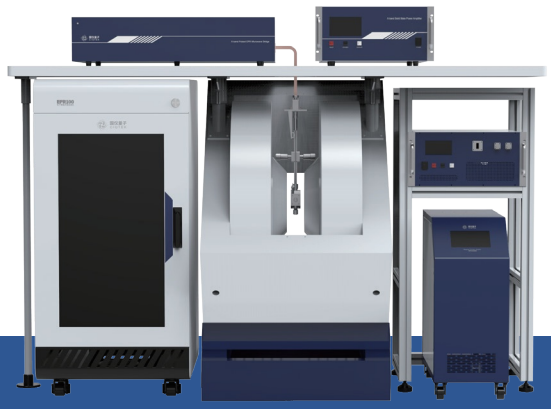

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Exploiting the EPR toolbox in copper(II) chemistry

S. Fardokht Rezayi,[1,2] Andrea Guidetti,[1,2] Damien M. Murphy,[2] Nóra V. May,[3] Norbert Lihi,[4] Sabine Van Doorslaer.[1]

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[2] School of Chemistry, Cardiff University, Park Place, Cardiff CF10 3AT, United Kingdom;
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[4] HUN-REN-UD, Department of Inorganic and Analytical Chemistry, Faculty of Science and Technology, University of Debrecen, H-4032 Debrecen, Hungary.

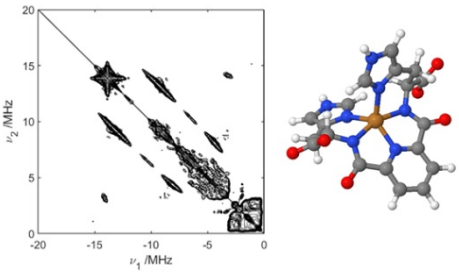

Figure 1: (left) X-band ^{14}N-HYSCORE of a Cu(II) pyridine-carboxamide complex at pH 12, highlighting the region of the contributions of the directly copper-coordinated ^{14}N of the His residues of the complex; (right) corresponding DFT structure of the Cu(II) complex.

Due to the crucial role that copper plays in many biological systems and chemical applications, in which the activity of the system is completely determined by the local geometry around the copper centre, there is a continuing interest in copper coordination chemistry. EPR has proven to be an excellent tool to study Cu(II)-complexes. A large fraction of the EPR studies has focused on octahedral, square planar or square pyramidal Cu(II) complexes with a $(d_{x^2-y^2})^1$ ground-state configuration. Surprisingly, far less attention has been devoted to the Cu(II) centres with trigonal pyramidal (tbp) geometry or with more distorted square-pyramidal local coordination, which also occur ubiquitously. Using a combination of density functional theory (DFT), multi-frequency field-swept EPR and a series of hyperfine spectroscopies, we here tackle a number of these less studied geometries. We first focus on the catalytic Cu(II) complex of tris(2-aminoethyl)amine (TREN), which undergoes pH-dependent geometry changes and adopts a tbp geometry at high pH. This structural change is reflected in the CW-EPR, ENDOR and HYSCORE spectra when compared to those of the square-pyramidal states. In a next part, we move to the study of Cu(II) pyridine-carboxamide complexes with superoxide dismutase activity that are potential drug candidates for the treatment of various diseases related to oxidative stress. While the CW-EPR spectra of these complexes are also pH-dependent, they remain more or less in line with what is normally ascribed to a $(d_{x^2-y^2})^1$ ground-state configuration. However, for some cases, hyperfine spectroscopy reveals a different story, with e.g. surprising ^{14}N HYSCORE features (Fig. 1) and related hyperfine parameters, that are also observed for the tbp Cu(II) TREN complex, but have not been reported for the 'standard' square (pyramidal) Cu(II) complexes. The talk will show that, after more than 80 years of EPR spectroscopy, EPR-analyses of homogeneous Cu(II) complexes may seem trivial, but hold many surprises.

[This work was partially funded from the European Union's Horizon 2020 research and innovation program (Marie Skłodowska-Curie Grant Agreement n° 813209)]

Investigating Protein Structure and Function Through Paramagnetic Substitution of Native Metal Ions

Katrin Ackermann, Bela E. Bode

EaStCHEM School of Chemistry, Biomedical Sciences Research Complex, Centre of Magnetic Resonance, University of St Andrews, North Haugh, St Andrews, KY16 9ST, Scotland

Electron Paramagnetic Resonance (EPR) spectroscopy is an important tool for structural analysis and characterisation of biomacromolecules that is not limited by the size, shape, or complexity of the system. The paramagnetic species EPR spectroscopy requires can be either endogenous, such as paramagnetic metal centres or cofactors, or deliberately introduced to the site(s) of interest. The latter is commonly achieved by incorporating stable nitroxide radicals via site-specific mutagenesis and site-directed spin labelling or by site-specifically engineering artificial metal ion binding sites. A further option that is explored in this contribution is substituting endogenous diamagnetic metal ions (e.g., Zn^{II}) with paramagnetic ones (e.g., Cu^{II}). Mammalian histidine-rich glycoprotein (HRG) is a glycosylated protein of ~70 kDa in size and is present in blood plasma at relatively high concentrations (~1.5 μM). It has numerous binding partners, such as heparin, plasminogen, divalent metal ions, and heme, and is involved in many essential regulatory biological processes, including blood coagulation, cell migration, proliferation and adhesion. It has therefore been referred to as the “Swiss Army knife of mammalian plasma”. In this contribution we showcase how a combination of continuous wave EPR, hyperfine and dipolar spectroscopies, and Cu^{II}-substitution of Zn^{II}-sites leads to assemble a holistic picture of native HRG and its interaction with metal ions.[1] Expanding to further plasma proteins we investigated Cu^{II}-binding to Human Serum Albumin (HSA) and can identify and affinity-rank copper ion binding sites by iterative histidine knockout mutations.[2] By investigating microbial nutrient import as a potential strategy for delivery of antibiotics a 2-site model has been suggested for ferric-enterobactin with its transporter from *Pseudomonas aeruginosa*.[3] By substituting the enterobactin-bound iron ion with vanadium we could obtain high quality pulse dipolar EPR data on the complex bound to its spin-labelled transporter. Experiments validating the crystallographic model in solution will be presented.[4]

[1] K. Ackermann, S. Khazaipoul, J. L. Wort, A. I. S. Sobczak, H. EL Mkami, A. J. Stewart, B. E. Bode, *J. Am. Chem. Soc.* **2023**, *145*, 8064.
[2] K. Ackermann, D. Wu, A. J. Stewart, B. E. Bode, *Dalton Trans*. **2024**, *53*, 13529.
[3] L Moynié, S. Milenkovic, G. L. A. Mislin, V. Gasser, G. Malloci, E. Baco, R. P. McCaughan, M. G. P. Page, I. J. Schalk, M. Ceccarelli, J. H. Naismith, *Nat. Commun.* **2019**, *10*, 3673.
[4] K. Ackermann et al. *unpublished data*.

Characterisation of a semiquinone radical bound in the active site of respiratory complex I by hyperfine EPR spectroscopy

Eleanor R. Clifford,[1] John J. Wright,[2] Alberto Collauto,[1] Judy Hirst,[2*] Maxie M. Roessler.[1*]

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[2] Medical Research Council Mitochondrial Biology Unit, University of Cambridge, Keith Peters Building, Cambridge Biomedical Campus, Cambridge CB2 0XY, UK.

Quinone reduction is a key step in catalysis by respiratory complex I (RCI), an essential energy-transducing enzyme that drives ATP synthesis by oxidative phosphorylation. However, the mechanism of quinone reduction and the role of semiquinone (SQ) intermediates in catalysis remain poorly understood. Previous spectroscopic investigations of SQ species have been complicated by difficulties in assigning the low-intensity g ~ 2 EPR signals observed using native membrane systems or non-native quinone substrates.[1,2]

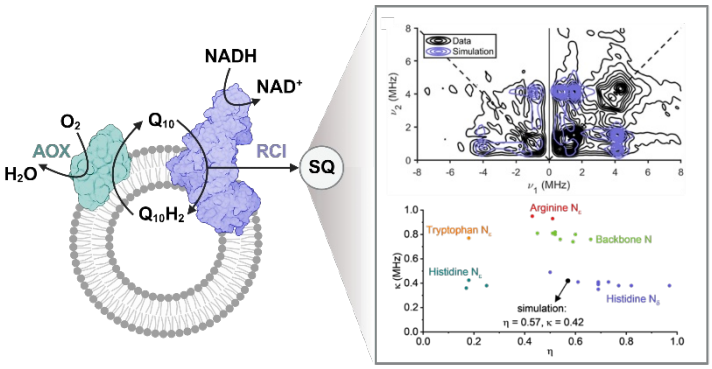

Figure 1: Investigation of a respiratory complex I semiquinone catalytic intermediate using a simple, native-like proteoliposome system. Pulse hyperfine EPR and simulation of the nuclear quadrupolar interaction identifies a hydrogen bond to the N_δ nitrogen of a conserved active site histidine residue.

Here, we employ a biochemically and spectroscopically 'clean' proteoliposome system[3] to investigate SQ formation by mammalian RCI in the absence of other respiratory proteins and using the native ubiquinone-10 (Q_{10}) substrate. Following addition of NADH, we observe a g = 2.005 signal and use continuous-wave EPR to assign it to a SQ radical bound at the top of the quinone-binding channel, close to iron-sulfur cluster N2, the terminal cluster in the chain that connects it to the NADH-binding site. Using an EPR probehead modified for investigation of low-intensity signals,[4] we then employ a hyperfine pulsed EPR technique (HYSCORE) to define the coordination environment of the semiquinone species, including a direct hydrogen bond with N_δ of a protonated histidine residue that we propose is the conserved active-site histidine essential for catalysis.

Our results shed light on the Q_{10} reduction reaction that is key to the mechanism of energy coupling in RCI, and demonstrate how pulsed EPR methods can provide detailed information on radical species formed in challenging energy-converting membrane proteins.

[1] Wright et al. BMC Biol., 2020, 10.1186/s12915-020-00768-6
[2] Hirst and Roessler, BBA – Bioenergetics, 2016, 10.1016/j.bbabio.2015.12.009
[3] Eisermann et al., Chem. Eur. J., 2024, 10.1002/chem.202402035
[4] Šimėnas et al., J. Mag. Res., 2021, 10.1016/j.jmr.2020.106876

EPR and HYSCORE spectroscopic characterisation of the coordination of the ferric thiolate haem cofactor in a *de novo* designed protein mimicking natural cyt P450 monooxygenases

Joshua S. Harbort,[1] Iago De Assis Modenez,[2] Guillaume Gerbaud,[1] Stéphane Grimaldi,[1] Vincent L. Pecoraro,[2] Anabella Ivancich.[1]

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[2] Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109, United States

Cytochrome P450 monooxygenases (P450s) are versatile haem thiolate catalysts that work through the controlled activation of inert C-H bonds under physiological conditions, a 'Holy Grail' of chemical synthesis. Site-directed mutagenesis on natural P450s has illustrated the importance of the haem iron's 2nd coordination sphere in modulating the function of P450 catalytic processes, with recent reports showing a single amino acid substitution converts P450 monooxygenases into efficient peroxygenases [1,2]. However, site-directed mutagenesis can also lead to undesirable allosteric effects and changes in hydrogen bond networks related to substrate binding and intramolecular electron transfer. We have thus chosen to exploit the *de novo* proteins design to obtain α-helical scaffolds with a cysteine binding site for the haem [3]. EPR and HYSCORE are powerful techniques to characterise the specific binding mode of the haem (axial ligand and distal side environment) in the *de novo* proteins. Substitution of well-chosen amino acid residues allows us to tailor the haem's 2nd coordination sphere to mimic structural and functional features of natural P450s. We have used cw and pulse EPR techniques (HYSCORE) to characterise mutants of the low-spin thiolate haem that were tailored to modify the pKa of the Cys16 axial ligand and the haem distal side (Fig. 1). The advantageous possibility of synthesising the *de novo* proteins with isotopically labelled amino acid residues (deuterated non-exchangeable protons, ^{15}N-labelled His or Lys) allowed us to unequivocally identify the ligands of the ferric haem cofactor. Fig. 1 shows the weakly-coupled proton and deuterium regions of the 9 GHz HYSCORE spectrum of the GRW-L16CL30H scaffold (in which the Cys16 β protons have been substituted with deuterium) in complex with haem and in deuterated buffer. The mutations modifying the pKa of Cys16 will be discussed.

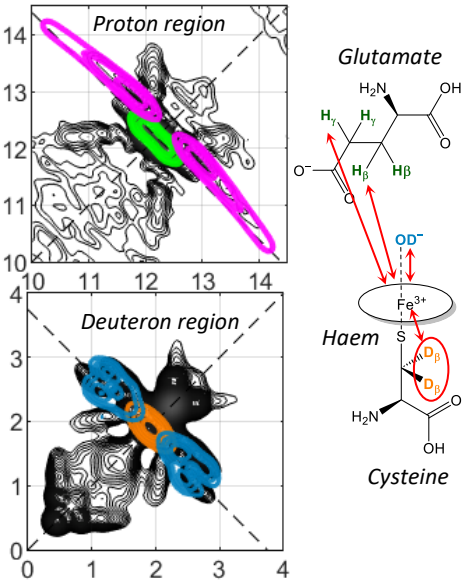

Figure 1: 9-GHz HYSCORE spectrum of the GRW-L16CL30H protein in complex with haem in deuterated buffer (pD 11) recorded at the g_Z field position of the ferric thiolate haem, using τ = 128 ns, T=12 K. The cross peaks detected in then deuterium region (which are no present in the control sample) clearly showed that Cys16 (in orange, narrow) and hydroxide (in blue, broad) are the ligands to the haem Fe^{3+}. Based on our protein sequence and our structural model, we propose that the non-exchangeable protons (green and magenta) arise from Glu27.

[1] Podgorski, M.N.; Lee, J.H.Z.; Harbort, J.S. *et al.*; *J Inorg Biochem*, (2023), **249**, 112391
[2] Podgorski, M.N. *et al.*; *ACS Catal*, (2025), **15**, 5191
[3] Koebke, K.J.; Kühl, T.; Lojou, E.; Demeler, B.; Schoepp-Cothenet, B.; Iranzo, O.; Pecoraro, V.L.; Ivancich, A.; *Angew Chem Int Ed*, (2021), **60**, 3974

EPR can follow electron hole hopping in proteins - but can we design new routes?

Dima Svistunenko,[1] Ben Skinner[1], James Birrell[1], Marina Lucic[1], Jonathan Worrall[1], Ethan Bungay[2], Holly Ford[2], Ross Anderson[2]

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Redox reactions in proteins and enzymes generate amino acid radicals, typically through one-electron oxidation followed by deprotonation. The resulting *electron hole* can be filled by an electron from a neighbouring residue, creating a new hole and promoting a through-protein hole hopping process. This process can be monitored by continuous wave (CW) EPR spectroscopy through following the free radical kinetics.

We will present a brief description of different EPR-based methods for determining the kinetics of paramagnetic species in biochemical reactions, including a) stopped-flow EPR in liquid phase; b) freeze-quenching samples at different time points after the reaction begins (including very short times); and c) different ways of freeze-quenching.

We will also show that an EPR spectrum change over reaction time requires a complex analysis. The free radical spectrum line shape always changes with reaction time (Fig. 1), but there could be different reasons for that.

It will be demonstrated that dye decolourising peroxidases (DyPs) provide an effective platform for analysing and designing new electron hole hopping routes in proteins [2].

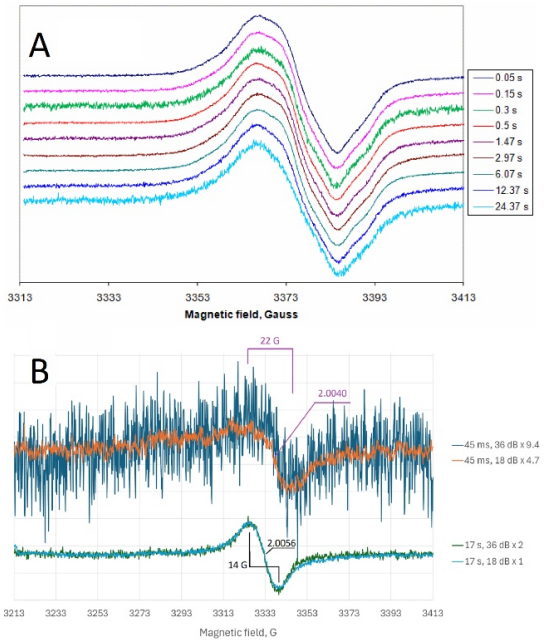

Figure 1: Free radical EPR spectra change over reaction time. **A** - Aplysia metMb + H_2O_2 [1], the spectra are normalized to the same intensity for convenient viewing of the spectral line shape; **B** - hexa-coordinate *de-novo* haem protein m4D2 + H_2O_2 . The common thing in many protein systems: with time, the free radical EPR signals become narrower and more isotropic.

The EHPath software [3] allows assessing the feasibility of hole hopping from one amino acid site to another, through redox active residues, and we will show that AlphaFold 3 [4] can generate models of DyP's variants, to be used sufficiently confidently as inputs for EPath, to predict new hole hopping paths in variants.

[1] B.J. Reeder et al. (2012) J Am Chem Soc, 134, 7741-9. 10.1021/ja211745g
[2] M. Lucic et al. (2023) Chem Sci, 14, 12518-34. 10.1039/d3sc04453j
[3] R.D. Teo et al. (2019) PNAS USA, 116, 15811-6. 10.1073/pnas.1906394116
[4] J. Abramson et al. (2024) Nature, 630, 493-500. 10.1038/s41586-024-07487-w

Progress and challenges in combining EPR & DFT for chemical insights into Ti(III)-based catalysts

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EPR & Hyperfine spectroscopy are powerful tools to study paramagnetic transition metal catalysts – particularly in combination with DFT calculations that facilitate the comparison of model structures to experimental data.

Established ENDOR techniques offer high spectral resolution, while suffering from low sensitivity when only a fraction of the nuclear spins can be excited. Here, using chirped RF excitation in chirp-ENDOR experiments, we show how sensitivity can be drastically increased, up to four times for ^{14}N and up to an order of magnitude for broad Cu(II) lines in a trade-off with spectral resolution.[1] To address complex samples that feature significant overlap in ENDOR spectra, we deconvolute the ENDOR spectra in a second, direct dimension via combination with chirp-echo detection. This CHEESY-ENDOR sequence allows to resolve overlapping lines from different nuclei in a hyperfine dimension as shown in Fig. 1 – without requiring significant additional measurement time because the ENDOR dimension remains the only indirect dimension, and we discuss applications and limitation of this experiment.

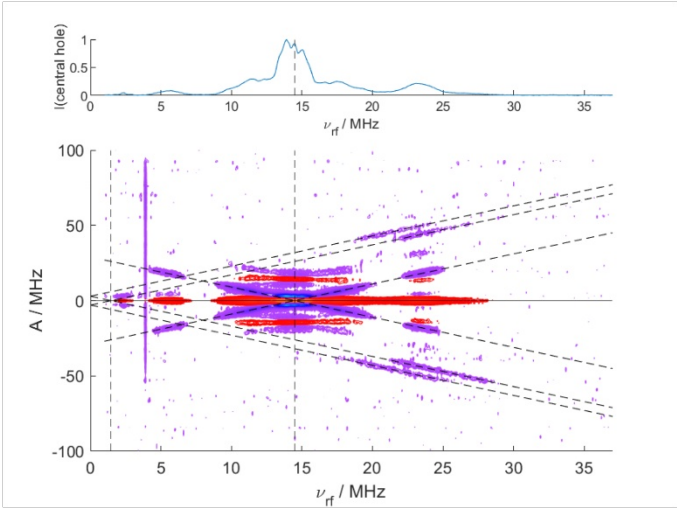

Figure 1: 2D CHEESY-ENDOR spectrum: ENDOR spectrum of a Cu(II) complex showing overlapping ^{1}H and ^{14}N peaks (top). Detection by chirp echo spectroscopy (CHEESY) enables deconvolution into 2D thus resolving the overlapping ENDOR resonances along a hyperfine axis as a second dimension (bottom).

For accurate comparisons of structures or models to experimental data accurate estimates and uncertainties for DFT-predicted g-tensors and hyperfine couplings are essential. Therefore, we combine experiments and calculations on well-defined molecular Ti(III) model complexes as a broader benchmark of our previous DFT protocols. The insights gained show accuracy improvements along with further potential. We show how combination of EPR & DFT clearly strengthens the data interpretation for both spectroscopic and DFT data, and thus enables more detailed mechanistic studies and offers chemical insight for widely applied transition metal catalysts.

[1] J. Stropp, N. Wili, N. C. Nielsen, D. Klose, *Magnetic Resonance* 6, 33-42 (**2025**) Increased Sensitivity in electron-nuclear double resonance spectroscopy with chirped radiofrequency pulses.

Conformational Dynamics and Asymmetry in Multimodal Inhibition of Membrane-bound Pyrophosphatases

Joshua L. Wort,[1] Xinyu Liu,[1] Yue Ma,[1] Anokhi Shah,[1] Keni Vidilaseris,[2] Adrian Goldman,[2] Christos Pliotas.[1]
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The integral membrane-bound pyrophosphatases (mPPases) are homo-dimeric Na^+/H^+ ion pumps that hydrolyse pyrophosphate (PPi) and are essential virulence factors in pathogenic protists. As such, mPPases are candidate therapeutic targets for small-molecule inhibitors, with particular focus on bisphosphonates. Herein, we use pulse electron-electron double resonance (PELDOR)[1] to probe the solution-state conformational ensemble of *Thermatoga* maritima mPPase (TmPPase) *apo*-state, in presence of various bisphosphonate inhibitors, and in presence of Ca^{2+} as an activator[2], validated by X-ray crystallography structural data.

Interestingly, we observed an apparent symmetry-breaking across the membrane between monomers of the constituent dimer – by measuring interspin distances on both the cytosolic (C599R1 and T211R1) and periplasmic (S525R1) membrane sides (Fig. 1). While the cytosolic side is consistent with an asymmetric 'closed-open' conformation (under most tested conditions), this does not fully propagate to the periplasmic side, which is instead most consistent with a symmetric 'open-open' conformation. This symmetry breaking is further supported by time-resolved X-ray crystallography,[3] solid-supported membrane electrophysiology measurements, and overlap coefficients (taken as a proxy for model agreement) between the 'open-open' conformation and S525R1 PELDOR distance distributions. This study demonstrates the potential utility of PELDOR to explore intramolecular asymmetries inherent to functional cycles of integral membrane proteins.

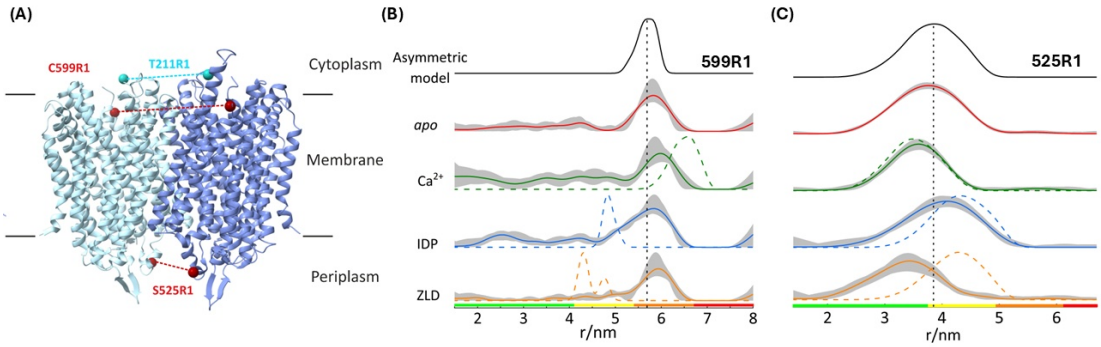

Figure 1: **(A)** TmPPase dimer structure and associated labelling sites. **(B, C)** PELDOR distance distributions under various conditions for 599R1 and 525R1 dimers, respectively. 95% confidence intervals (CI) are shown as shaded regions, and dashed lines are in-silico distributions predicted from symmetric X-ray crystal structures. The colour-bars indicate the reliability of the probability density distribution according to DeerAnalysis2022.

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Native and Photo-induced Paramagnetic Species in Carbon Nitride Photocatalysts

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Heterogeneous inorganic (photo)catalysts find application in a wide range of technologically relevant processes because of their stability and recyclability. They usually consist on high-surface area solid materials that either bind active species such as metals or directly generate active species through, for instance, photoexcitation.

Carbon nitride (CN) is an important class of heterogeneous photocatalysts, which has attracted considerable research interest since its first demonstration of photocatalytic H_2 production in 2009. Further research, motivated by their tunable band gap, chemical stability and structural flexibility, has shown that CN materials are competent towards many chemical reactions. Furthermore, metal ions can be firmly bound to nitrogen-rich coordination sites in CN, making them a unique class of hosts for preparing single-atom catalysts (SACs).

The understanding of the photocatalytic performance of CN is limited by an under-developed mechanistic understanding of the photodriven interfacial electron transfer and of all the intermediates formed after photoexcitation.

In this contribution I will show how – by exploiting their magnetic properties – Electron Paramagnetic Resonance (EPR) spectroscopy provides fundamental information on the local structure, spatial distribution and electronic structure of key intermediates even in this structurally disordered material.

The wealth of information derived from the whole array of EPR techniques are integrated to gain a comprehensive description on the photophysics and (photo)chemistry of native and photo-generated paramagnetic species in CN.

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EPR investigation of anionic vacancies: semiconductor physics and heterogeneous catalysis

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Point defects are of extreme importance in determining the physical and chemical properties of materials. Among these, anionic vacancies are particularly crucial for semiconductors, as they can induce a completely different magnetic, optical and electric properties, compared to an ideal vacancy-free material. This is largely due to the introduction of intra-bandgap states and electron-donor behaviour associated with vacancies formation. At the same time, anionic vacancies in heterogeneous catalysts have an important role in many chemical reactions, such as CO_2 to MeOH conversion [1-3] and NH_3 oxidation.[4]

As for many point defects, the detection of anionic vacancies is often not trivial. EPR is a powerful method for their investigation, as vacancies often act as electron trapping sites (F-centers) and become paramagnetic. Here we present a general view on oxygen vacancies from a semiconductor physics perspective and the implications for catalysis, based on *operando* EPR results on a series of reducible oxides (In_2O_3, CeO_2, ZrO_2 and others). The effect of reducibility, bandgap and external doping are considered. It is shown how the formation of oxygen vacancies can lead to an increase of n-type conductivity, decrease of p-type conductivity, how they can act as electron trapping sites and how all these phenomena can be investigated by EPR. In this context, the formation of a defect band at high vacancies density, leading to exchange-coupled vacancy-bound polarons with distinct EPR features is discussed

The investigation of nitrogen vacancies in carbon nitrides are also presented, as an example of a combination of *operando*, CW and pulse EPR methods (ESEEM and RIDME), together with DFT, providing a deep understanding of their reaction-induced structural changes and contribution to the catalytic behaviour of the material.

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High-Field Dynamic Nuclear Polarization in Liquids: Toward Biomolecular Applications

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The solid effect in Dynamic Nuclear Polarization (DNP) has gained renewed attention in the field of liquid-state Nuclear Magnetic Resonance (NMR). Traditionally, it was believed that the solid effect was only effective in solid-state environments, particularly at high magnetic fields. However, recent investigations have broadened this perspective, revealing its potential for hyperpolarizing nuclei in the fluid phase of lipid bilayers [1] and viscous liquids [2, 3].

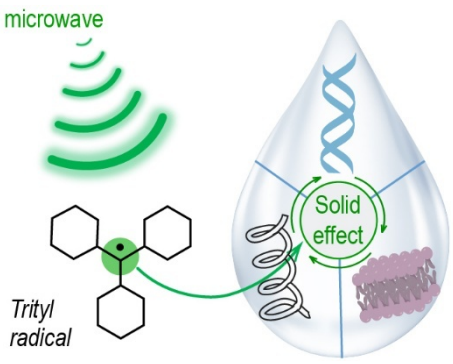

Figure 1. Schematic illustration of the solid-effect DNP methodology for studying biologically relevant molecules. This approach enables the investigation of peptides, adenosine triphosphate, nucleic acids, and cellular membranes at high magnetic fields and within nanoliter sample volumes, enhancing sensitivity in NMR spectroscopy.

This study expands the applicability of solid-effect DNP, demonstrating its efficiency even in aqueous solutions at room temperature. We report a remarkable DNP enhancement exceeding 20-fold for adenosine triphosphate, oligonucleotides and DNA dissolved in water. Significant enhancements were achieved for both proton and phosphorus nuclei at a magnetic field of 9.4 T on the nanoliter scale [4]. These results highlight the capability of solid-effect DNP to enhance NMR signal, particularly in studying biomolecular dynamics and non-covalent binding interactions under physiologically relevant conditions.

This work was supported by the DFG grant (Deutsche Forschungsgemeinschaft, No. 518679424).

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Population transfers in a molecular 4f qudit

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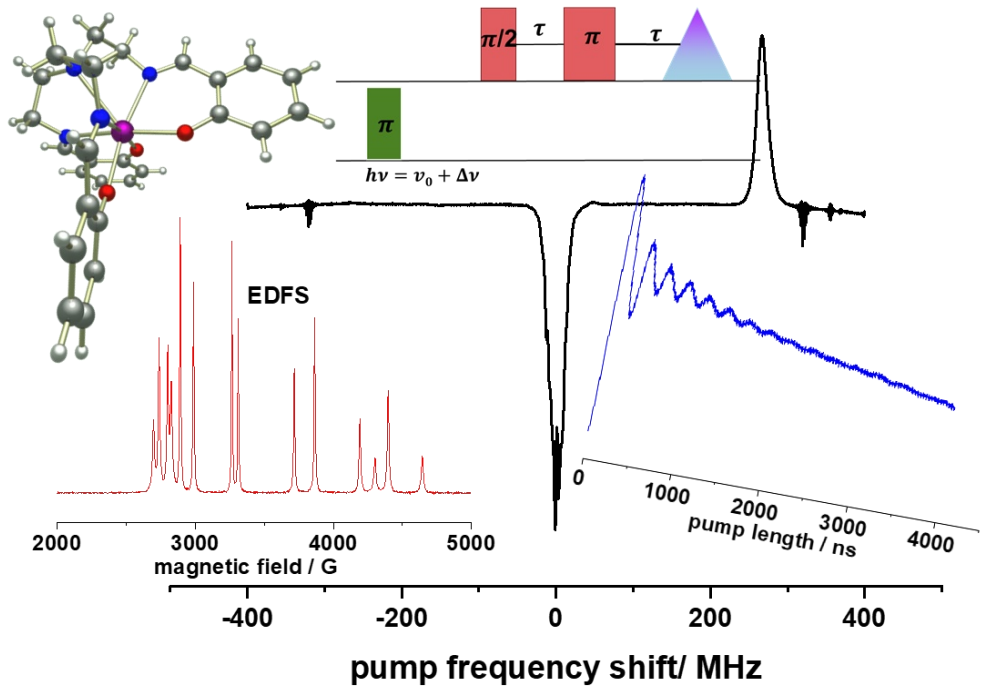

Figure 1: Population transfer in Gd(trensal).

In recent years we have shown that molecular 4f coordination complexes hold potential for use in Quantum Technologies.[1,2,3,4,5] In particular, the multilevel structure of Gd(III) in Gd(trensal) allows for the implementation of a molecular 8-level qudit or of 3 qubits. We recently probed the fundamental factors that induce decoherence in ensembles of such molecular qudits by X-band pulse EPR on single crystals of Gd@Y(trensal) at 0.5, 10^{-1} , 10^{-2} and 10^{-3} % doping levels.[6]

To go beyond simple coherent manipulation of molecular spins such as single qubit rotations, the ability to coherently manipulate more than two angular momentum states in a single pulse sequence, is required. We demonstrate herein that population transfer between the states of the 8-level Gd(III) qudit is achievable (Figure 1).

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From charge-transfer states to separated charges: organic photovoltaics probed by transient and pulse EPR

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Recent advances in the design of non-fullerene acceptors, paired with organic polymer donors, have propelled efficiencies of organic photovoltaics towards 20%, however, a clear understanding of the underlying photophysical processes that contribute to the light-to-electricity conversion is still missing and of paramount importance for further improvements in performance.[1] The charge-transfer state (a weakly-coupled radical pair) and separated charges are key intermediates and both contain unpaired spins; they can be selectively probed by light-induced EPR spectroscopy.

The EPR spectral signatures of separated charges on the polymer donor and non-fullerene acceptor were characterised by echo-detected EPR performed at multiple frequencies to provide enhanced resolution of *g*-anisotropy. Since the donor and acceptor signals overlap considerably, even at W-band, we employed a number of pulse EPR techniques to distinguish the two contributions. We selectively probed coupled ^{14}N nuclei unique to the non-fullerene acceptor using ELDOR-detected NMR, and exploited differences in spin relaxation in inversion recovery experiments.[2]

We then carried out a detailed transient EPR study to characterise the initial charge-transfer state for a series of donor:acceptor blends, varying temperature and laser fluence to explore the relationship between the properties and dynamics of the photogenerated states and device efficiency. Shortly after photoexcitation, all blends exhibit a characteristic charge-transfer state signal, that evolves into a predominantly absorptive feature at longer times. Simulations reveal a broad distribution of spin environments, and differences in molecular ordering. Accurate modelling of the evolution of spin polarisation required including an equilibrium between the charge-transfer state and separated charges. These insights provide a deeper understanding of charge separation and recombination, linking molecular-scale interactions to macroscopic device performance.

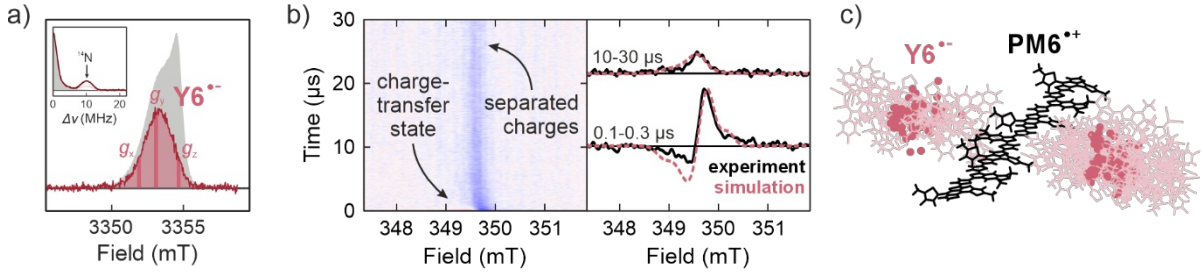

Figure 1: a) W-band ELDOR-detected NMR-induced EPR spectrum of Y6; b) X-band transient EPR spectrum of PM6:Y6 with simulation using the stochastic Liouville equation; c) Ordering of PM6 and Y6 molecules at the donor:acceptor interface, extracted from simulation of the 0.1-0.3 μs charge-transfer state signal.

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Frequency and time domain ^{19}F ENDOR spectroscopy: role of nuclear dipolar couplings to determine distance distributions

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^{19}F electron-nuclear double resonance (ENDOR) spectroscopy is emerging as a method of choice to determine molecular distances in the angstrom to nanometre range. [1] Especially the structure of biomolecules is often flexible and thus a distribution of distances is present, resulting in multiple spin-dipolar couplings. This correlates to a broadening of the line width in frequency domain ENDOR spectra. [2]

However, other line broadening mechanisms in ^{19}F ENDOR spectra can obscure the distance information, thus limiting both the resolution and the accessible distance range.

Here, the investigation of the broadening mechanisms is presented. For this a combination of rational molecular design, frequency and time domain ENDOR methods as well as quantum mechanical spin dynamics simulations are applied. [3]

The nuclear dipolar couplings between the fluorine and protons up to 14 kHz are identified as a major source of spectral broadening. They could be removed by H/D exchange, resulting in reduction of the spectral width to 9 kHz.

The identified strategies can then be applied to the analysis of ENDOR spectra of a spin labelled RNA duplex. There, the spectral ENDOR line width could be predicted, which in turn enabled the extraction of a distance distribution (see Fig. 1), thereby representing a first step towards a quantitative determination of distance distributions in biomolecules from ^{19}F ENDOR.

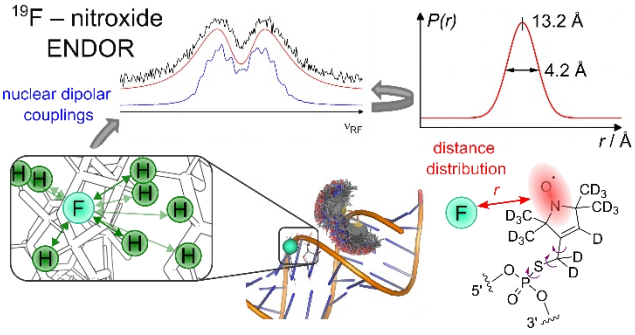

Figure 1: Nuclear dipolar couplings to protons contribute significantly to the line broadening observed in frequency domain ^{19}F ENDOR spectra and need to be considered for the analysis of distance distributions.

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Direct Detection of the Chirality Induced Spin Selectivity Effect in Donor Acceptor Molecules

Hannah J. Eckvahl,[1] Nikolai A. Tcyrulnikov,[1] Alessandro Chiesa,[2] Graeme Copley,[1] Jillian M. Bradley,[1] Ryan M. Young,[1] Stefano Carreta,[2] Matthew D. Krzyniak,[1] Michael R. Wasielewski[1]

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Chirality induced spin selectivity (CISS) can polarize electron spins as they transfer through a chiral molecule[1], however previous investigations had only been done while molecules were bound to a substrate. Here, we experimentally investigated the effect of chirality on donor acceptor molecules (D-B$_X$-A) using time resolved electron paramagnetic resonance spectroscopy (trEPR) in two different systems by comparing them to their achiral analogues.

In the first system, a series of D-B$_X$-A molecules, shown in Figure 1a, were synthesized. Selective photoexcitation of D induces a sub nanosecond two-step electron transfer process to form D$^{\bullet+}$-B$_X$-A$^{\bullet-}$, which was then studied using trEPR. When aligned perpendicular to the external magnetic field, the chiral molecules exhibited line shape changes that are characteristic of the CISS effect with a CISS contribution of about 47%[2]. In the second system, shown in Figure 1b, selective photoexcitation of A induced a sub nanosecond two-step hole transfer to form D$^{\bullet+}$-B$_X$-A$^{\bullet-}$. trEPR measurements in a glassy solvent without orientation showed changes in the line shape that were characteristic of the CISS effect with a CISS contribution of about 38%[3].

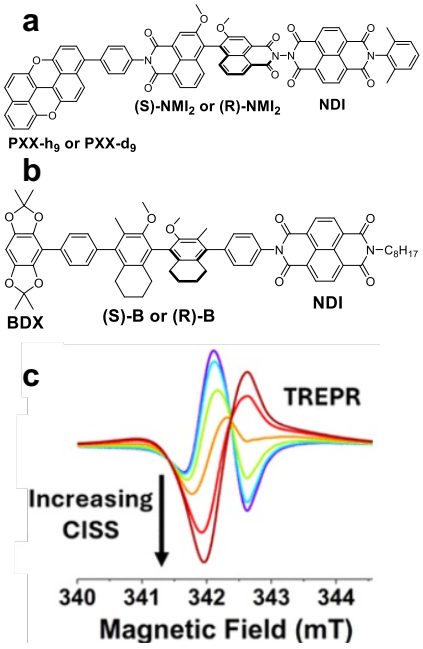

Figure 1 a) First chiral system in which the D is either non-deuterated (h$_9$) or deuterated (d$_9$) in which both the R and S enantiomer of B$_X$ was studied. b) Second chiral system in which both the R and S enantiomer of B$_X$ was studied. c) Simulation of trEPR spectra of the second chiral system with increasing CISS contribution.

These were the first experiments to demonstrate the CISS effect at the molecular level. They are complementary experiments that demonstrate that i) the CISS effect influences the spin dynamics of donor acceptor systems when both electron transfer and hole transfer occur and ii) the CISS effect can be directly detected with EPR spectroscopy. We are currently working on new model systems to further investigate the role of chirality in the spin dynamics of donor acceptor molecules.

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Exploiting Spins in Molecular Semiconductors – from Solar Cells to Quantum Technologies

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Polyaromatic molecules play a key role in next-generation energy devices. In addition to the low thermal budget involved in processing, their applications range from energy-harvesting in e.g. flexible solar cells, to low-energy operation in e.g. organic light emitting devices and unconventional computing. The photophysical properties of the materials also enable unique generation and utilisation of electronic spins, which are attractive in quantum applications, including communication and sensing.

This presentation will consider pentacene as the archetypal molecular semiconductor thin film, and focus on the structure-property relationship of spin-based properties. This will firstly involve singlet fission, which can boost the performance of solar cells by generating two charges for every photon absorbed in neighbouring pentacene molecules [1]. The mechanism of fission is interpreted via molecular film design coupled to electron spin resonance spectroscopy [2], and temperature-dependent spectroscopy [3], with perspectives for utilising the initial state of fission in quantum information and computing [4]. In isolated pentacene molecules, the spin-polarised triplet states can be harnessed in a range of applications, and the potential of pentacene films for quantum-enhanced sensing is considered [4]. Finally, new design approaches to exploit spin in hybrid structures for improved photovoltaic performance are presented [5].

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Zero-field Splittings in Metalloarsinidene and Organobismuthinidene Studied by FD-FT THz-EPR

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Subvalent main group compounds, with oxidation states lower than their normal group oxidation state, frequently form highly reactive, transient triplet states, as crucial reaction intermediates. Progress in the stabilization of main group triplet states paved the way for their in depth characterization. EPR has been successfully employed to study light main group triplet states, like e.g. carbenes or nitrenes. However, very little is known about the magnetic properties of the heavier homologues.

Here, we report on the EPR characterization of two heavy group 15 triplet states: a palladiumarsinidene formed through photolysis at cryogenic temperatures[1] and the first stable organobismuthinidene.[2] Triplet EPR spectra are dominated by zero-field splitting (ZFS), originating from dipolar and spin-orbit coupling. Since the latter scales with the atomic number, ZFS in heavy elements easily exceeds the excitation energy in conventional EPR spectrometers (e.g. 0.3 cm^{-1} (X-band) or 3 cm^{-1} (W-band)). To determine the ZFS of triplet states whose energies span several orders of magnitude, we therefore use Frequency-Domain Fourier-transform THz EPR spectroscopy (FD-FT THz EPR). The employed THz-EPR set-up has an exceptional wide detection window from 3 cm^{-1} to 6000 cm^{-1}, with the option of light excitation in the sample magnet at cryogenic temperatures. Our approach enabled the determination of ZFS in the heavy triplet pnictinidenes providing fundamental insight into the magnetic properties and electronic structure of this important class of compounds.

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Wideband techniques in HF EPR

Graham Smith,[1] Yujie Zhao[2], Rob Hunter[1], Daniel Sung[1], Hassane El Mkami[1]:

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High frequency EPR and DNP spectrometers operating in the high mm-wave and sub-mm-wave regime often use a combination of quasi-optical techniques to provide large bandwidth, and low loss components and transmission. The term "quasi-optical" itself refers to using a combination of single-mode and over-moded techniques and the HIPER pulsed EPR spectrometer [1] is an example of this methodology. This spectrometer operates with very large excitation and detection bandwidths whilst providing extremely high isolation between transmitter, detector and the sample-holder. This combination provides fast response times, very low deadtime and very high concentration sensitivity, as well as compatability with DNP and ENDOR measurements. The recent integration of a fast AWG also now allows precise excitation over extended bandwidths (>1 GHz).

In this talk I will discuss a number of enabling quasi-optical technologies, and a specific integration of a wideband AWG (Agilent M8190A) that makes use of digital IQ upconversion (Figure 1). This offers wide instantaneous bandwidths with very low levels of spurii, low memory usage and fully coherent detection, which can provide compensation for phase drift. In the talk I will give examples that showcase many of the advantages associated with this type of implementation.

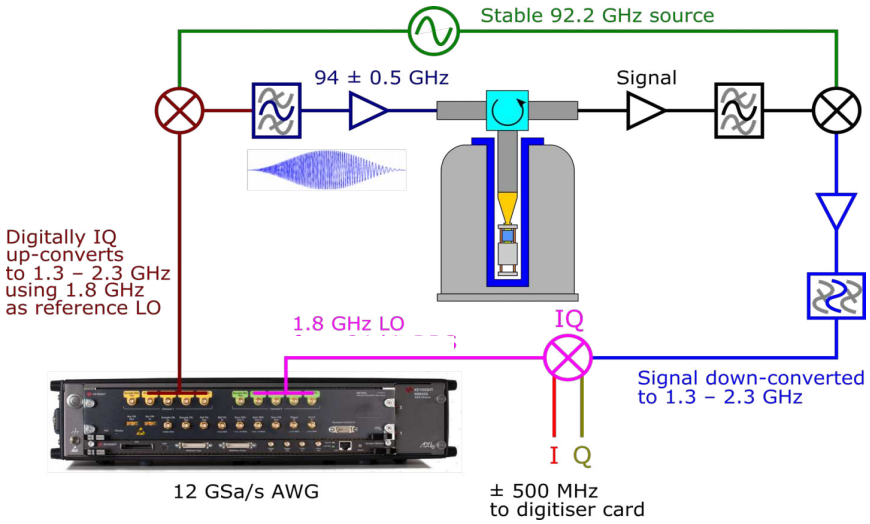

Figure 1 The AWG implementation in the HIPER spectrometer makes use of digital upconversion to reduce memory usage, reduce spuria and harmonics whilst allowing for considerable flexibility in permitting fully coherent detection at offset frequencies.

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A monosubstituted C(0) atom in its triplet state: expanding the family of carbon-centered diradicals

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Among carbon-centered diradicals, carbenes—featuring a disubstituted carbon atom—form the most extensively studied class, which found applications in various fields of chemistry. In contrast, monovalent carbon compounds are largely underrepresented. Recent advances in organic synthesis[1, 2] have enabled us to pursue novel classes of triplet-state molecules, such as triplet vinylidenes.[3]

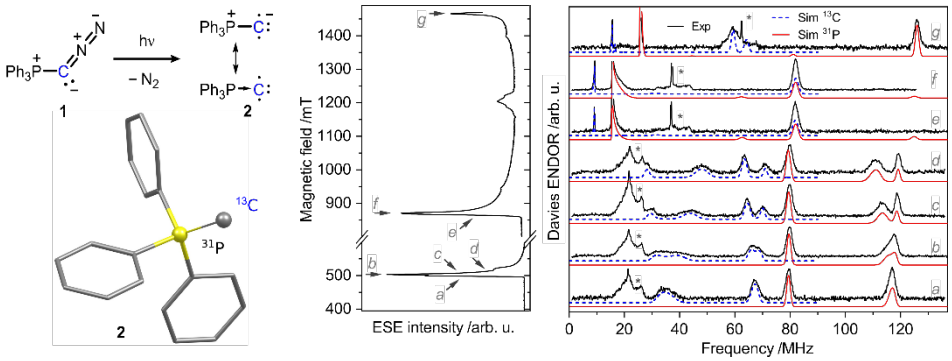

Figure 1: Photogeneration of the triplet-state $Ph_3P{\rightarrow}C$ (**2**) from the diazophosphorus ylide **1** (top left); quantum chemical model of **2** (bottom left); Q-band EPR spectrum of **2** (middle); ^{13}C and ^{31}P ENDOR spectra of **2** recorded at the marked field positions with simulations (right).

Here we present an EPR/ENDOR characterization of $Ph_3P{\rightarrow}C$[4], a novel compound photochemically generated from the recently synthesized diazophosphorus ylide Ph_3PCN_2[5] (Fig. 1, left).

A triplet ground state of this monovalent diradical species was elucidated by multi-frequency/temperature-dependent EPR spectroscopy (Q-band data in Fig. 2, middle). A positive ZFS parameter $D = +0.543\ cm^{-1}$ and a vanishingly small rhombicity $|E|/D = 0.002$ were obtained from spectral simulations. Since the D value is in the range typical for some carbenes, orientation-selective ENDOR (Fig. 1, right) was used to constrain the electronic structure based on the purely axial ^{13}C and predominantly isotropic ^{31}P HF tensors.

The P−C bond is best described as dative. The bonding can be understood in terms of a triplet C atom in its ground ^3P state (arising from the $2s^22p^2$ configuration) accepting the lone pair from Ph_3P, which straightforwardly explains the triplet ground state of the monovalent carbon adduct.

[1] Varava, P. et al. *Nature Chemistry.* 2021, 13, 1055–60.
[2] Antoni, P.W. et al. *Nature Chemistry.* 2021, 13, 587–93.
[3] Kutin, Y. et al. *J. Am. Chem. Soc.* 2021, 143, 21410–5.
[4] Kutin, Y. et al. *Angew. Chem. Int. Ed.* 2025, 64, e202424166.
[5] Koike, T. et al. *Science.* 2024, 385, 305-11.

Bright Triplet and Charge-Separated Singlet Excitons in Organic Diradicals Enable Optical Addressability of Spin States.

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The ability to optically initialize and read-out spin states is pivotal for quantum technologies, with applications in quantum computing, communication, and sensing. Molecular systems are a promising quantum platform due to their reproducibility, chemical versatility, and precise geometric and spatial control achievable through accessible synthetic chemistry. Among these, spin radical organic semiconductors show exceptional potential, as they can exhibit high luminescence [1, 2] and spin-dependent luminescence via high-spin states [3].

Here, we report a fully organic diradical system comprising two chlorinated trityl (TTM) units connected via a meta-linked fluorene bridge, which exhibits spin-dependent luminescence with near-unity photoluminescence quantum yield [4].

Electron paramagnetic resonance (EPR) spectroscopy reveals a triplet dark ground state, and transient EPR measurements indicate spin-sublevel selective intersystem crossing, with ground-state polarization persisting up to 200 μs at 200 K. Coherent spin control is demonstrated using pulsed EPR, while optical initialization and read-out are achieved through optically detected magnetic resonance (ODMR) [4]. The exceptional combination of high luminescence, localized spin character, and coherent addressability positions this diradical system as a compelling new platform for optically controllable molecular spin semiconductors with potential applications in quantum information processing and sensing.

[1] Ai X., *et al.*, Nature, **2018**, 563, 536
[2] Cho H. *et al.*, Advanced Materials, **2023**, 35, 2303666
[3] Gorgon S. *et al.*, Nature, **2023**, 620, 538
[4] Chowdhury R., Murto P., Panjwani N. A., *et al.*, **2024**, arxiv.org/abs/2406.03365

High-Spin State Dynamics and Quintet-Mediated Emission in Singlet Fission Systems

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High-spin states are crucial in various organic applications, spanning from optoelectronics to quantum information and singlet fission (SF). This talk focuses on the formation and emission of quintet and triplet states in SF systems. The principle is based on a photoexcited singlet exciton rapidly decaying into spin-correlated triplet pairs, forming singlet, triplet and quintet states, before dissociating into free triplets (Fig. 1). While extensive studies have addressed triplet formation and its role in photoluminescence, emission pathways involving quintet states remain largely unexplored. Additionally, strategies to tune SF systems for controlled triplet multiplication via molecular design are still of high interest. We employ a set of unique spin-sensitive techniques to investigate high-spin state formation and emission, including optical spectroscopy, such as transient absorption (TA) and magnetic field dependent photoluminescence (magPL), as well as electron paramagnetic resonance (EPR) and optically detected magnetic resonance (ODMR).

We focus on novel concepts of intramolecular and intermolecular singlet fission based on units of the SF-active chromophore diphenylhexatriene (DPH). A particular focus will be on DPH-based oligomers, which allow tuneable geometry for accessing different spin regimes [1]. We show that quintet states form robustly across architectures and, remarkably, mediate delayed photoluminescence even at room temperature, as confirmed by ODMR. However, the efficiency of triplet separation is highly dependent on the number of chromophores and molecular arrangement. These findings offer a general framework for controlling high-spin dynamics in organic materials, relevant for both exciton multiplication and optically addressable spin states.

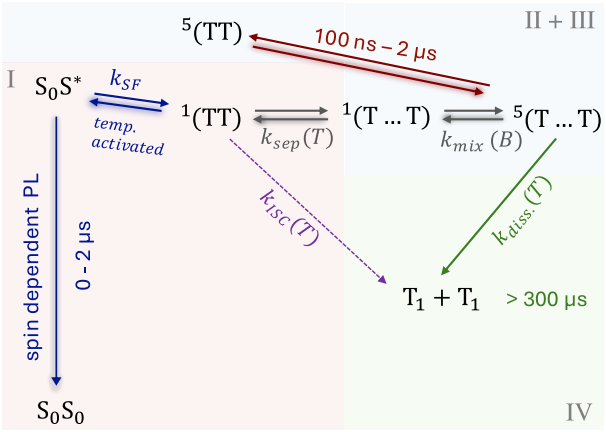

Figure 1. Spin-sensitive techniques monitor the involvement of different spin states in intra- molecular singlet fission.

[1] Grüne, J., Montanaro, S., Bradbury, T.W., et. al. 2024. High-Spin State Dynamics and Quintet-Mediated Emission in Intramolecular Singlet Fission. *arXiv preprint arXiv:2410.07891*.

Harnessing the Potential of Spectroelectrochemical EPR: Design and Application

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Spectroelectrochemical EPR (SEC-EPR) is a powerful tool that combines electrochemistry and electron paramagnetic resonance, offering unparalleled insights into redox processes and paramagnetic species. The multifaceted advantages of SEC-EPR are highlighted by its versatility in various applications such as determining active sites in oxygen reduction reactions (ORR) and identifying and characterizing radicals in redox reactions [1]. Its application extends beyond in-situ analysis to operando conditions, allowing for the acquisition of key mechanistic information on catalytic systems. SEC-EPR integrates seamlessly with other spectroscopic techniques, such as Mössbauer spectroscopy, providing clarity and support. It can be used to investigate redox materials of all sizes, from small molecules like nitroxides to larger redox-active proteins [2]. The intricate design aspects of SEC-EPR are crucial for optimising performance and accuracy, underscoring that these considerations are far from trivial [3]. By showcasing innovative design strategies and practical examples ranging from large commercial spectrometers to benchtop to homemade EPR-on-a-Chip (EPRoC), the full potential as well as the future of SEC-EPR are demonstrated.

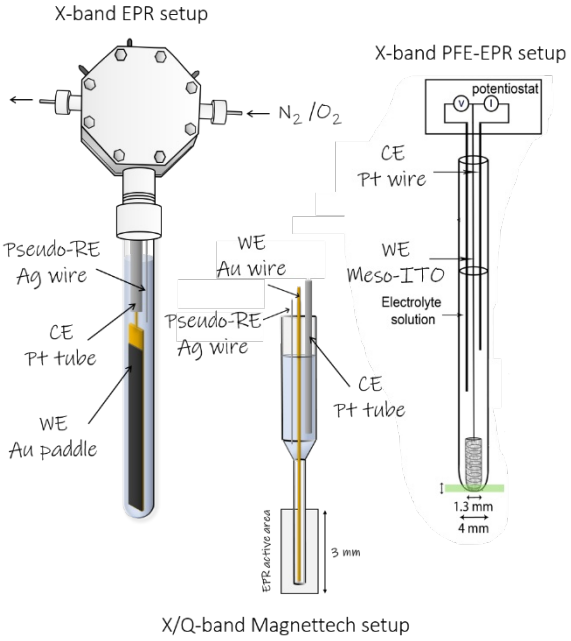

Figure 1: SEC-EPR setups for in-situ X-band commercial setups such as ELEXSYS-II and Magnettech and Q-band EPR spectrometer.

[1] Kagilev, Alexey A., et al. "The power of in situ spectroelectrochemistry for redox study of organometallic and coordination compounds." Journal of Solid State Electrochemistry 28.3 (2024): 897-910.
[2]Abdiaziz, Kaltum, et al. "Protein film electrochemical EPR spectroscopy as a technique to investigate redox reactions in biomolecules." Chemical Communications 55.60 (2019): 8840-8843.
[3] Seif-Eddine, Maryam, et al. "Operando film-electrochemical EPR spectroscopy tracks radical intermediates in surface-immobilized catalysts." Nature Chemistry 16.6 (2024): 1015-1023.

A Tale of Two Light-induced EPR Experiments

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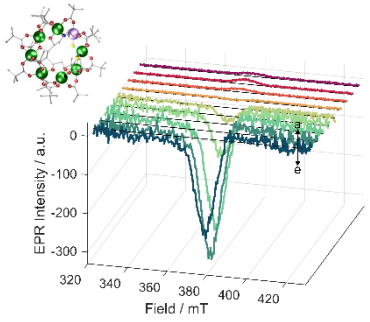
Light-induced Electron Paramagnetic Resonance (LiEPR) shows great promise in both structural determination of biological systems and in controlling spin populations in multi-metallic macromolecular systems which may have potential pathways for implementation of quantum gates.

Applications of LiEPR methods in biological systems have opened up possibilities for using chromophore-based triplet-labels that can be directly compared to Förster Resonance Energy Transfer (FRET) using the same labels,[1] and using combinations of selective microwave pulses [2] with polarisation of light [3] to afford orientation selective measurements. The analysis of these measurements must include consideration of the underlying biological structure, which is possible by combining Maximum Entropy based methods with Molecular Dynamics (MD) simulations.[4]



In materials systems, antiferromagnetically coupled heterometallic rings, and {Cr_7Ni} rings in particular, have been long studied as potential molecular qubits, as two-level systems with agreeable phase memory times for application of gate operations.[5] These systems have additionally been proven as flexible tools for building multi-qubit systems [6] and successfully employed in supramolecular constructs with redox-switchable linkers.[7] The possibility to use light to switch these systems is a novel application and we present an investigation of the light-induced behaviour of different Cr-based antiferromagnetically coupled heterometallic systems (see figure).[8]

[1] J. Am. Chem. Soc. 2023, 145, 42, 22859–22865; [2] J. Phys. Chem. Lett. 2021, 12, 15, 3819–3826; [3] Phys. Chem. Chem. Phys. 2024, 26, 28398-28405; [4] In preparation; [5] Phys. Rev. Lett. 2005, 94, 207208; [6] Inorg. Chem. 2024, 63, 15460; [7] Chem. 2016, 1, 727; [8] In preparation.

Single spin magnetic resonance by microwave photon counting

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France

Pushing magnetic resonance spectroscopy to the single-spin level is a long-standing objective in both ESR and NMR, with far-reaching implications for materials science, chemistry, and nanoscale sensing. In this talk, I will present recent advances that enable the detection and coherent manipulation of individual electron and nuclear spins in a solid-state crystal using microwave fluorescence and superconducting quantum bits. I will begin by describing how single-electron spin resonance spectroscopy is achieved on individual erbium ions embedded in a $CaWO_4$ crystal at millikelvin temperatures, using a superconducting resonator to enhance radiative relaxation and a single-microwave-photon detector for readout [1]. Building on this platform, I will then show how hyperfine-coupled 183W nuclear spins can be identified, monitored in real time via quantum jumps, and read out in single-shot measurements [2]. Finally, I will introduce a new all-microwave protocol based on stimulated Raman driving, which enables both single- and two-qubit operations between nuclear spins, as well as the preparation of entangled states with coherence times exceeding one second [3]. These results define a robust and scalable framework for single-spin ESR and NMR, relying exclusively on microwave control and detection, and are broadly compatible with a wide range of paramagnetic systems.

[1] Z. Wang et al., "Single-electron spin resonance detection by microwave photon counting," *Nature* 619, 276–281 (2023).
[2] J. Travesedo et al., "All-microwave spectroscopy and polarization of individual nuclear spins in a solid," *Science Advances* 11, (2025).
[3] J. O'Sullivan et al., "Individual solid-state nuclear spin qubits with coherence exceeding seconds," *arXiv:2410.10432* (2024).

Solid-State Maser with Microwatt Output Power at Moderate Cryogenic Temperatures

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[1] Schulich Faculty of Chemistry, Technion – Israel Institute of Technology, Haifa, 3200003, Israel

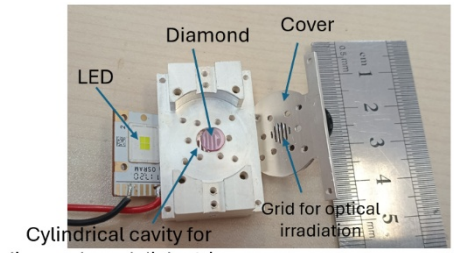

Figure 1: Photograph of the maser resonator in its open state.

Solid-state masers are uniquely positioned to serve as ultra-low phase noise microwave sources due to their exceptionally low noise temperatures. However, their practical application has been historically limited by low output power and the need for deep cryogenic cooling. In this work, we present a novel design for a continuous-wave diamond-based maser oscillator employing the energy levels of electron spins in nitrogen-vacancy (NV) colour defects. This maser operates at a static field of ~0.6T at ~14.5 GHz and moderate cryogenic temperatures (~180 K), and achieved output power levels exceeding –30 dBm (1 μW). This performance represents a two-orders-of-magnitude improvement over previous diamond or ruby-based maser oscillators. Our system integrates a high-Q (~2460) compact metallic microwave cavity with optically pumped [111]-oriented NV-rich diamond crystals (Fig 1). The cavity supports efficient light coupling and thermal dissipation, enabling sustained high-power optical excitation (>1 W) using cost-effective green LEDs. We demonstrate stable maser operation with good spectral quality and validate its output through both frequency- and time-domain analysis with phase noise data when operated in “free running” mode. Additionally, we provide phase noise estimations based on Leeson’s model and show that, when coupled to a high-Q external resonator, such masers could approach thermally limited phase noise levels. These predictions suggest strong potential for diamond masers to outperform traditional ruby-based or similar maser systems, especially given their ability to operate at higher temperatures using rugged, He-free Stirling coolers. Despite current limitations related to frequency stability and jitter, this work establishes diamond-based masers as promising candidates for next-generation ultra-low phase noise microwave oscillators. Further engineering optimization—particularly in field stability, thermal regulation, and feedback locking—will be key to unlocking their full potential.

Utilizing optimal magnetic field configurations for mitigating decoherence in optical spin defects

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[5]SIAS, Krea University, Sri City 517646, India

Mitigating decoherence in optical spin qubits is a crucial challenge in advancing varied quantum technologies. In this work, we present a comprehensive study to suppress decoherence in spin-1 electronic systems. Specifically, focusing on the negatively charged boron vacancy center in hexagonal boron nitride (hBN), we explore the role of static magnetic field strength and orientation in attaining decoherence-free subspaces. Using detailed numerical simulations of the spin Hamiltonian, we identify specific magnetic field configurations that minimize energy gradients and curvatures. Furthermore, we develop an approximate analytical model based on perturbation theory to predict these low-gradient subspaces, providing a generalized framework applicable to a variety of spin-1 systems. These results are significantly valuable for defect-based quantum sensing applications. Furthermore, we extend our analysis to telecom-band emitters, including nitrogen vacancy centers in silicon carbide and G-centers in silicon. We investigate coherence properties and identify optimal conditions for enhanced coherence in these systems. These findings are particularly relevant for long-distance quantum communications as these systems are well compatible with the existing fiber-optic infrastructure.

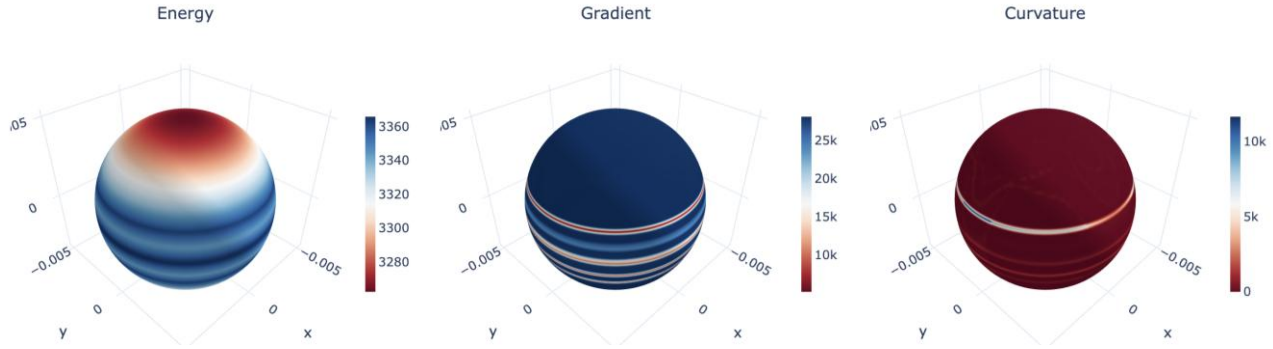

FIG. Transition energy, gradient, and curvature— evaluated as functions of the polar and azimuthal angles of a 5.1 mT bias magnetic field for one of the most probable spin transitions within the ground-state triplet manifold of the negatively charged boron vacancy center in two-dimensional hexagonal boron nitride.

Surface-Ensemble Electron Spin Resonance of Ultra-Thin YPc_2 Films as a Potential Molecular Spin Qubit Architecture

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[2]Ewha Womans University, Seoul, 03760, Republic of Korea
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Molecule-based spin qubit architectures are promising for quantum computing due to their chemical tunability and long coherence times [1]. Among these, yttrium phthalocyanine double-decker (YPc_2) stands out due to its magnetic properties, which are primarily attributed to an unpaired electron (S = 1/2) delocalized on the Pc ligand [2]. In addition, this molecule is generally found to adsorb flat and self-assemble on single crystal surfaces [3]. These characteristics make YPc_2 a promising building block for spin qubit architecture and at the same time an ideal benchmark for surface-ensemble electron spin resonance (ESR) experiments [4].

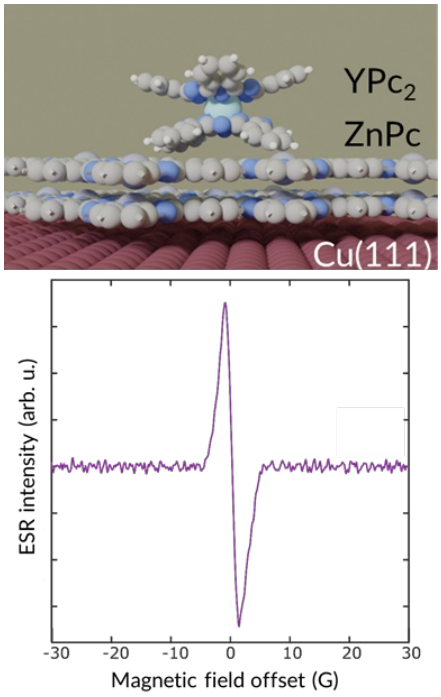

Figure 1: Top: Schematics of the molecular multilayer YPc2 / ZnPc / Cu(111) vertical heterostructure. Bottom: X-band ESR signal of 6 layers of YPc_2 on 10 layers ZnPc obtained with the custom-built surface-ensemble spectrometer [4] at room temperature after background subtraction.

Here, we investigated the morphology, electronic structure, and spin properties of single- and multi-layer YPc_2 on Cu(111) single crystals and on zinc phthalocyanine (ZnPc) grown on Cu(111). Low temperature scanning tunneling microscopy allows us to determine the structure of the molecular layer and the variation of its electronic configuration when directly adsorbed on Cu(111) versus on a ZnPc decoupling layer. X-band ESR performed in ultra-high vacuum with our custom-built surface-sensitive spectrometer [4] shows that the radical spin of YPc_2 is preserved on ZnPc while being quenched upon direct contact with Cu(111). Density functional theory attributes this quenching to the hybridization of molecular orbitals with the substrate electrons. Our study validates the potential of YPc_2 / ZnPc heterostructures to realize molecular spin qubit architecture, provided the spin is decoupled from the metallic substrate.

[1] Fursina, A. A., et al. ACS Appl. Electron. Mater., 2023, 5(6), 3531.
[2] Branzoli, F., et al. Phys. Rev. B, 2011, 83(17), 174419.
[3] Zhang, Y., et al. Nano Res., 2010, 3(6), 604-611.
[4] Cho, F. H., et al. Rev. Sci. Instrum., 2024, 95(6), 063904.

Hyperpolarizing ^{209}Bi:Si nuclear spins using superconducting microresonators

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[2] London Centre for Nanotechnology, UCL. (UK)
[3] Electrical and Computer Engineering, Princeton University. (USA)
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Bismuth donors in silicon provide an ideal platform for a quantum memory, allowing random access state retrieval [1] and up to 3s coherence times [2]. Superconducting microresonators patterned on top of donor spins allow high sensitivity readout and efficient control of the spin system and provide and an ideal pathway to couple the memory to a quantum processor [3]. We show how a nearby waveguide can be used as an RF antenna to drive nuclear spins in the donor system and use it to perform ENDOR measurements on the bismuth nuclear spins, operating close to a ZEro-First-Order-Zeeman (ZEFOZ) point within the system. Experiments done at 100mK allow total polarization of the electron spin but leave very long spin lattice relaxation times. The large Q factor and small mode volume of the superconducting resonator leads to a Purcell enhanced decay rate for resonant spins. The short T1 along the resonant transition and manipulation of the nuclear spin allows combination of spin populations from different nuclear spin states (fig. 1), hyperpolarizing the spins.

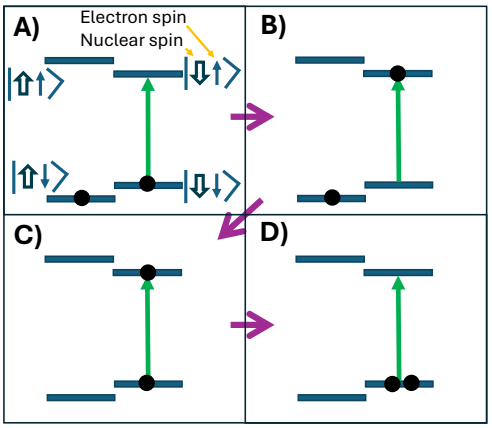

Figure 1: Proposed hyperpolarisation scheme. A) Nuclear spin states start with equal populations; electron spin is completely polarised. B) Spins resonant with microresonator are inverted (π_e). C) Nuclear spins are inverted (π_n). D) Purcell enhanced T1 causes spins to preferentially decay along resonant transition, combining populations.

[1] O'Sullivan, J. et al. *Physical Review X* **12**, (2022)
[2] Wolfowicz, G. et al. *Nature Nanotechnology* **8**, 561–564 (2013)
[3] Kubo, Y. et al. *Physical Review Letters* **107**, (2011)

Superconducting spiral microresonators enable versatile high sensitivity EPR

Gediminas Usevičius,[1], Blaise L. Geoghegan,[2] Oscar W. Kennedy,[3] Ignas Pocius,[1] Patrick Hogan,[3] Ana Villanueva Ruiz de Temino,[3] Jean-Baptiste Verstraete,[3] Paulina Verbaitytė,[1] Angeliki Chatziathanasiou,[2] G. Antilen Jacob,[3] Joseph Alexander,[3] Vidmantas Kalendra,[1] Jūras Banys,[1] Maxie M. Roessler,[2] John J.L. Morton,[3,4], Mantas Šimėnas[1]

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We present a three-orders of magnitude increase in the spin number sensitivity of X-band pulsed EPR in a manner which is fully compatible with conventional instrumentation and typical sample conditions, up to fields exceeding 1 T and temperatures up to 80 K. Our approach employs planar spiral-shaped microresonators of 7 nL mode volumes fabricated from Yttrium Barium Copper Oxide (YBCO) high-temperature superconductor. We achieve a wide range of microwave coupling by placing a single microresonator inside a conventional EPR tube, loaded into an EPR cavity (Figure 1). The performance of the spiral microresonators is demonstrated through a suite of pulsed EPR experiments on standard samples including DEER, ESEEM, and ENDOR. By placing a sample within a microfluidic microstructure fabricated to match the mode profile of the microresonator, we obtain a high-fidelity spin control with a spin-number sensitivity of 10^7 spins/G/√Hz. Our approach significantly advances the applicability of superconducting microresonators as versatile and readily applicable tools for high sensitivity EPR.

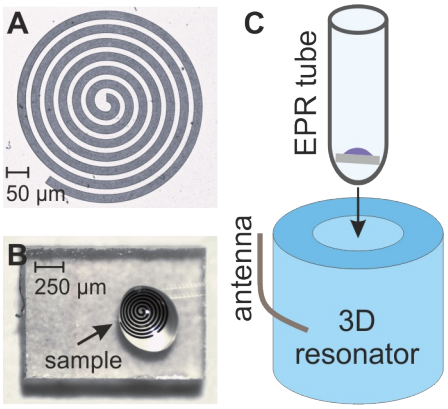

Figure 1: (a) Fabricated planar YBCO spiral microwave microresonator on a sapphire substrate. (b) Individual microresonator with an aqueous droplet containing nitroxide radicals. (c) The microresonator sits approximately horizontally at the bottom of an EPR tube, which is then loaded into a standard 3D EPR resonator facilitating coupling to a microwave antenna.

autoDEER – Fully Automated DEER Spectroscopy

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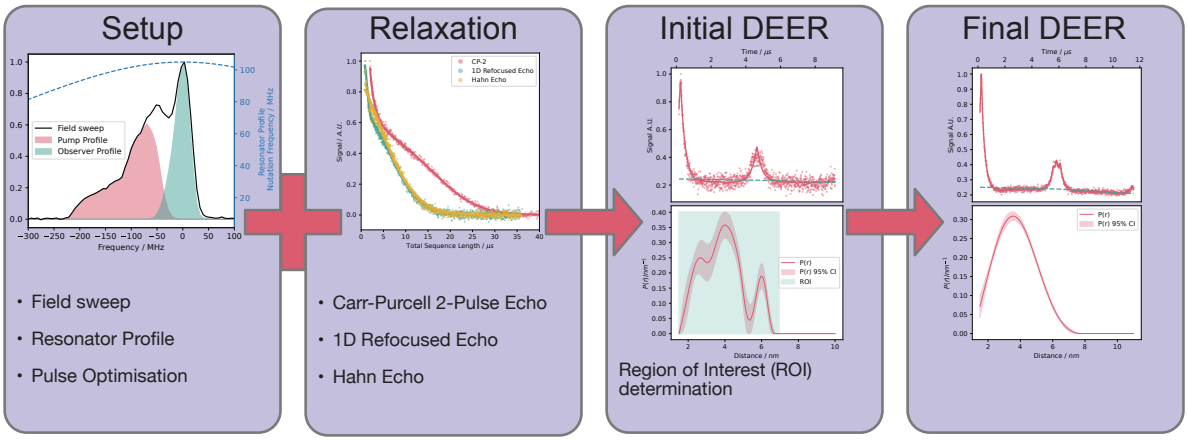

Here we present autoDEER, a Python-based add-on software to existing pulse EPR spectrometers that provides a fully automatic implementation of a rigorous protocol for highly optimised DEER measurements using nitroxide spin labels. This protocol determines whether 4-pulse or 5-pulse DEER are better for the given spectrometer, sample and time constraint, and tunes the pulse sequence parameters including pump and observe frequencies, pulse shapes, and inter-pulse delays.

The autoDEER graphical user interface (GUI) provides two operating modes: a “fully automatic mode” requiring minimal user input, and an “advanced mode” providing control over specific parameters such as pulse type, sequence type and inter-pulse delays whilst still benefiting from partial automation. Real-time data visualisation, analysis and fitting provides immediate feedback during experiments.

We have rigorously validated autoDEER and the underlying protocol against a wide range of published samples ranging from simple short and rigid proteins to highly flexible intrinsically disordered proteins. Both protonated and deuterated matrices have been tested.

Released under the GPL-3.0 open-source license, autoDEER’s code and protocol are fully transparent, enabling community-driven development and adaption to the latest developments.

The source code, documentation and other resources are available at github.com/JeschkeLab/autoDEER and jeschkelab.github.io/autoDEER.

Electron spin resonance at the nanometre scale using diamond quantum sensors

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Quantum sensors can enable the probing of electron spin resonance (ESR) and nuclear magnetic resonance signals in nanoscale volumes[1,2]. Such spatial resolution, reaching the scale of single molecules, allow the targeting of free radicals in biological and chemical environments, without needing to average over large sample volumes. For example, nanoscale sensing of reactive oxygen species (ROS) could help inform the design of next generation fuel cell devices, which typically suffer from membrane degradation driven by ROS. In living systems, ROS are crucial to cell signalling and healthy cell operation, but their presence can also be an indicator of stress and of disease onset. In high concentrations, ROS also cause damage to DNA.

Diamond nanocrystals containing nitrogen-vacancy (NV) colour centres can harness quantum phenomena to perform a variety of sensing tasks such as measuring temperature, viscosity and external magnetic and electric field, at the nanoscale, even inside live cells[2-4]. These quantum sensors can operate without suffering from bleaching and are unaffected by changes in local pH and local refractive index, remaining robust to fluctuations in background fluorescence. Through microwave spin manipulation that targets both the NV spin and radicals of interest, the NV spin can act as an ESR device, probing its immediate nanoscale vicinity. In this talk, I will discuss nanodiamond-based quantum sensing in living systems and its applications in nanoscale ESR.

[1] Holzgrafe et al. Nanoscale NMR spectroscopy using nanodiamond quantum sensors. Phys. Rev. Appl. **13** 044004 (2020)

[2] Belser et al. 2023 Opportunities for diamond quantum metrology in biological systems`, *Appl. Phys. Lett.* **123** 020501 (2023)

[3] Gu et al., Simultaneous Nanorheometry and Nanothermometry Using Intracellular Diamond Quantum Sensors *ACS Nano* 2023 **17** 20034−20042 (2023)

[4] Shanahan et al. Q-BiC: A Biocompatible Integrated Chip for in vitro and in vivo Spin-Based Quantum Sensing *PRX LIFE* **3** 013016 (2025)

Low-field magnetic clock transition of near-surface ^{75}As spins in silicon via electrically detected magnetic resonance

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Heavy group-V donor spins in silicon represent a promising avenue to realise a silicon-based quantum processor incorporating atomic scale qudits [1].

For donors with $I > 1/2$, the prominent electron-nuclear spin mixing in the intermediate field regime leads to the presence of clock transitions that can decouple the spin from sources of environmental magnetic field noise leading to long coherence times [2,3].

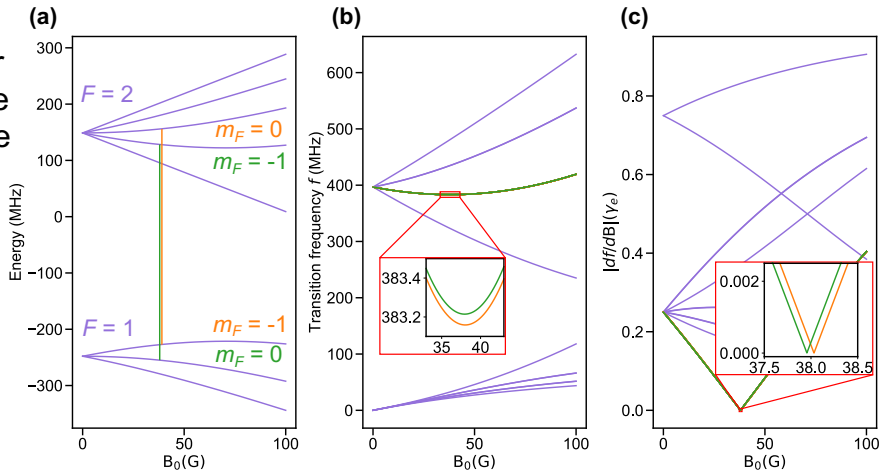

Figure 1. Low-field ^{75}As Breit-Rabi diagram. (a) Donor eigenstates with the pair of transitions composing the magnetic clock transition shown in orange and green. (b) Transition frequencies against field. The inset shows the turning points of the clock transition doublet. (c) The absolute value of the first derivative of the transition frequency with respect to the magnetic field in units of the electron gyromagnetic ratio (γ_e). The inset zooms into the clock transition doublet.

Here we map out the electron spin resonance magnetic field clock transition of an ensemble of near-surface (~ 20 nm) ^{75}As spins in ^{28}Si using low-field (<100 G) continuous wave electrically detected magnetic resonance. Here a resonant conductivity change is detected via a spin-dependent recombination pathway introduced by the formation of a near-surface spin-pair formed between the donor electron and the P_{b0} dangling bond found at the Si/SiO_2 interface. Linewidth broadening of the clock transition in the magnetic field domain is observed with quantitative analysis indicating the presence of strain within the micro-fabricated device employed for the measurement.

[1] Fernández de Fuentes et al., *Nature Communications*, 15(1), 1380, 2024.
[2] Wolfowicz et al., *Nature Nanotechnology,* 8(8), 561-564, 2013.
[3] Mohammady et al., *Phys Rev B*, 9(85),094404, 2012.

Spin mixing in supramolecular light-induced multi-spin systems

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Supramolecular chemistry utilises intermolecular interactions for the design of highly ordered complex structures or molecular devices, which is especially valuable in nanotechnology and could potentially be exploited for quantum information science (QIS).[1]

Assemblies consisting of an organic chromophore, a linker and a radical, are excellent model systems to investigate structure property relationships in light-induced multi-spin systems, which recently receive increased attention due to their exceptional properties and their potential for applications in molecular spintronics, including QIS.[2-4] Light excitation generates a triplet state at the chromophore site, which may then interact with the stable organic radical, leading to spin mixing and the formation of high-spin (quartet) states.[2]

This study, combines the two fields of supramolecular chemistry and molecular spintronics by exploring the properties of hydrogen-bonded chromophore–radical pairs, shown in Fig. 1. While titration experiments verify 1:1 binding with high association, the transient EPR data confirm quartet state formation and thereby efficient spin mixing through the triple-hydrogen-bonding motif. The results demonstrate that supramolecular chemistry may be exploited for exploring, developing and scaling up materials for QIS.[1]

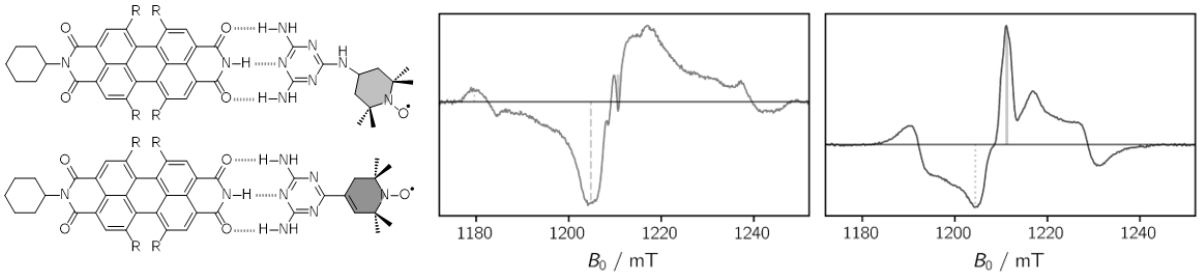

Figure 1: Structures of the investigated hydrogen-bonded chromophore–radical pairs and their EPR spectra.

[1] Khariushin, I. V.; Thielert, P.; Mayländer, M.; Zöllner, E.; Quintes, T.; Richert, S.; Vargas Jentzsch, A. *Nat. Chem.* **2025**, 17, 493–499.
[2] Quintes, T.; Mayländer, M.; Richert, S. *Nat. Rev. Chem.* **2023**, 7, 75–90.
[3] Mayländer, M.; Thielert, P.; Quintes, T.; Vargas Jentzsch, A.; Richert, S. *J. Am. Chem. Soc.* **2023**, 145, 25, 14064–14069.
[4] Mayländer, M.; Chen, S.; Lorenzo, E. R.; Wasielewski, M. R.; Richert, S. *J. Am. Chem. Soc*. **2021**, 143, 7050–7058.

In-cell EPR: A Combined Approach Using Nitroxide Radicals, SDSL and EPR to Probe Protein Behaviour within Cells

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[2] Department of Chemistry, University of Konstanz, Konstanz, Germany;
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Understanding how the intracellular medium modulates protein structural dynamics and protein-protein interactions is an intriguing but required topic scientists search to address by studying biomolecules in their native environment. As the cellular environment cannot be reproduced in vitro, investigation of biomolecules directly inside cells has attracted a growing interest in the past 20 years. Indeed, efforts in magnetic resonance spectroscopies have enabled important improvements in the study of structural dynamics directly in the cellular context.
Among magnetic resonances approaches, site-directed spin labeling coupled to electron paramagnetic resonance spectroscopy (SDSL-EPR) has demonstrated to be one of the powerful approaches to study structural properties of biomolecules.[1] In particular, nitroxide-based SDSL-EPR couples the benefits of high sensitivity and the lack of size constraints for the biomolecule of interest with the ability to study protein structural transitions and interactions at physiological temperature. [2,3,4,5]
In this talk, we will focus on the tools and strategies currently available to investigate cytosolic proteins and their interactions within cells by SDSL-EPR. Moreover, we will overview recent developments and highlight the main future research directions in the field.

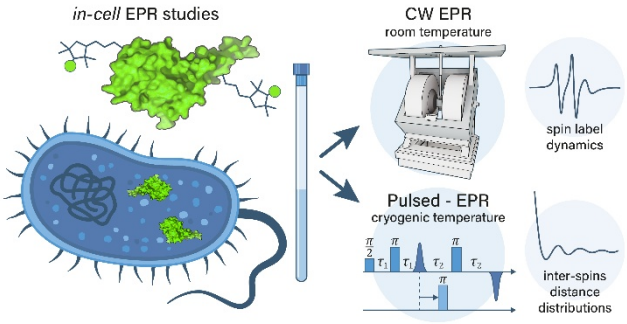

Figure 1: Schematic overview of a nitroxide-labelled protein studied within cells by EPR spectroscopy.

[1] A. Pierro, A. Bonucci, A. Magalon, V. Belle, E. Mileo. *Chemical Reviews* **2024**, 124 (17), 9873.
[2] G. Karthikeyan, A. Bonucci, G. Casano, G. Gerbaud, S. Abel, V. Thomé, L. Kodjabachian, A. Magalon, B. Guigliarelli, V. Belle, O. Ouari, E. Mileo, *Angew. Chem. Int. Ed.* **2018**, 130, 1380.
[3] A. Pierro, A. Bonucci, D. Normanno, M. Ansaldi, E. Etienne, G. Gerbaud, E. Pilet, B. Guigliarelli, O. Ouari, A. Magalon, V. Belle, E. Mileo, *Chem. – Eur. J.* **2022**, 28, e202202249.
[4] A. Pierro, K. C. Tamburrini, H. Leguenno, E. Etienne, G. Gerbaud, B. Guigliarelli, V. Belle, B. Zambelli, E. Mileo, *iScience*, **2023**, 26 (10), 107855.
[5] Y. Ben-Ishay, Y. Barak, O. Ouari, A. Pierro, E. Mileo, X.-C.-Su and D. Goldfarb* *Protein Science*, **2024**, 33(3), e4903.

^{19}F ENDOR as a means to determine the orientation of zero-field splitting tensor in Gd(III) chelates

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Orientation-selective electron-nuclear double resonance (ENDOR) in systems with resolved g-anisotropy is an essential source of structural information. This is possible because the orientation of the g-tensor principal axes in the molecule is usually known (e.g., nitroxides, Cu^{2+}, and VO^{2+} complexes). This approach, in principle, could also be applied for systems where the EPR powder pattern is determined by the zero-field splitting (ZFS), in particular, for high-spin half-integer systems, like Gd^{3+} and Mn^{2+}, which are commonly used probes in EPR. Unfortunately, in practice this approach has not been applicable, particularly for Gd(III), because of the extensive distribution of the ZFS in frozen solutions and the unknown orientation of the ZFS in the molecules.

This work presents a methodology that makes Gd(III) ZFS orientation selection approach possible. We first employ ^{19}F ENDOR to determine the ZFS molecular orientation in two commonly used Gd(III) spin labels. Using fluorinated model Gd(III) complexes with rigid and well-defined structures, based on a Gd(III) chelate frequently used in spin-labeling, we recorded ENDOR spectra on high-m_S electron spin transitions. Simulations of these spectra yielded the orientation of the ^{19}F-Gd vector in the ZFS principal frame, described by the polar (γ) and azimuthal (ρ) angles (Figure 1). However, this does not provide the full orientation of all three ZFS axes. To complete the picture, we used a second model compound with the same chelate but with the F at a different position. This combination yielded – for the first time – the orientation of the principal axes of the ZFS in the molecular frame, obtained from the frozen solution spectra. Finally, we show how this approach can be used to extract the structural information beyond the Gd(III)-^{19}F distance in Gd- and F-labeled proteins.

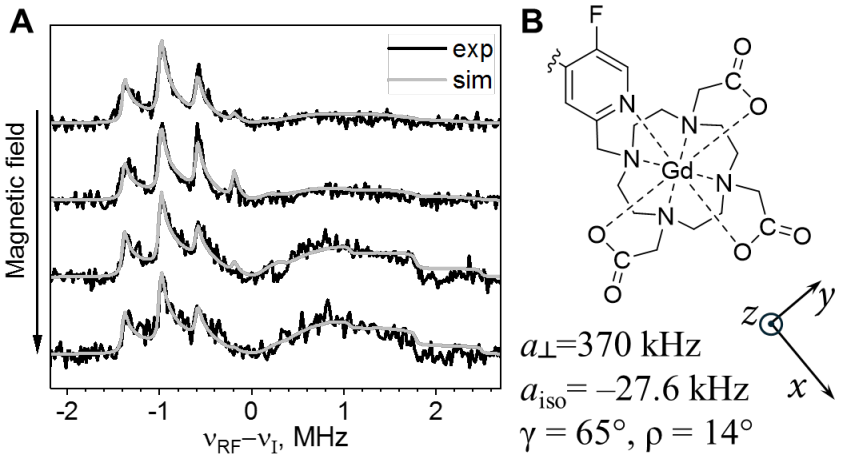

Figure 1: (A) Experimental (black) and simulated (gray) magnetic field dependence of ^{19}F ENDOR spectra of a Gd-DO3A complex featuring orientation selection and (B) the scheme showing the principal axes of Gd(III) ZFS,, experimentally determined from the spectra of a set of fluorinated Gd-DO3A derivatives, and the geometrical parameters obtained from the simulation.

Rotamer library analysis and investigations of the properties of the Bromoacrylaldehyde Spin Label

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Electron paramagnetic resonance (EPR) spectroscopy has proven to be a powerful tool for investigating the structure and dynamics of proteins in biological systems. Since most proteins are diamagnetic, the introduction of a paramagnetic probe is necessary, making the acquired information highly dependent on the properties of the spin probe. In this study, we present a rotamer analysis and a comparative investigation of the nitroxide-based Bromoacrylaldehyde Spin Label (BASL) [1] on two proteins, Bid and γD-crystallin. Using double electron-electron resonance (DEER) spectroscopy and continuous-wave EPR, we highlight the advantages of BASL over commercially available spin labels such as Methanethiosulfonate spin label (MTSSL) and Maleimido proxyl (MAP). We also demonstrate how BASL's surface specificity can be leveraged for orthogonal labeling strategies. Furthermore, the distances predicted by the rotamer library show good agreement with experimental DEER results and reveal narrower distance distributions compared to MTSSL. Finally, we underscore the advantageous properties of BASL as a direct backbone reporter and a viscosity-sensitive nanoprobe.

[1] Heaven G., Hollas M.A., Tabernero L., Fielding A.J., Spin Labelling of Surface Cysteines Using a Bromoacrylaldehyde Spin Label, Applied Magnetic Resonance 2021, 52 (8), 959-970.

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Host-guest complexes of various nitroxides as potential contrast agents for OMRI applications

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[2] Aix Marseille Univ., CNRS, ICR, UMR 7273, Case 551, Avenue Escadrille Normandie-Niemen, 13397, Marseille Cedex 20, France;

The Earth Field Overhauser-enhanced Magnetic Resonance Imaging (EF-OMRI) is developed as a relatively new and promising imaging technique that aimed to enhance the sensitivity and quality of MRI scans, by exploiting the enzyme/protease activity associated with various diseases and pathologies in different organs and tissues [1]. The use of nitroxide compounds is limited compared to traditional MRI contrast agents, but we aim to test their host-guest complexes as potential contrast agents.

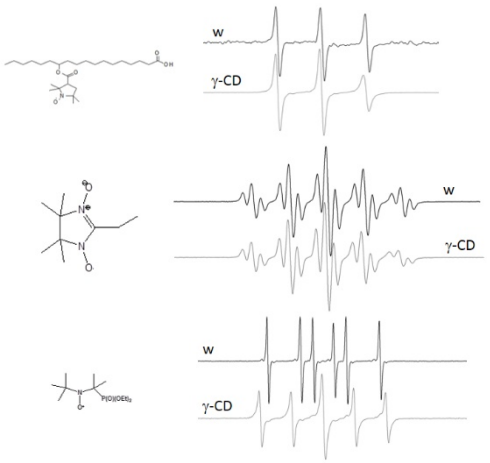

Figure 1: The EPR spectra of nitroxide, nitronyl nitroxide and β-phosphorilated nitroxide in water (black) and γ-cyclodextrin (grey)

In this study we examine the changes of EPR parameters of nitroxides, nitronyl nitroxides and their pair's imino nitroxides or β-phosphorylated nitroxides due to formation of host-guest complexes with cyclodextrins or cucurbiturils. Host-guest complexation may assure their protection against bio-reductants. While in the case of nitroxides the variation of aN values upon complexation is less than 1 G, in the case of nitronyl nitroxides, imino-nitroxides or b-phosphorylated nitroxides the changes in a_N or a_P values are higher, in some cases revealing significant change in the spectral shape [2].

[1] A. Comment, A. Perálvarez-Marín, Applications of Overhauser-enhanced magnetic resonance imaging (OMRI) in preclinical research. Antioxidants, 2019, 8(12), 625.
[2] A. V. F. Neculae, G. Audran, S. Bourdillon, G. Ionita, J. P. Joly, S. R. A. Marque, I. Matei, S. Mocanu, Conformational changes in β-phosphorylated nitroxides – A powerful tool to probe host–guest interactions, J. Mol. Liq. 2022, 364, 119983.

Acknowledgments: Project PNRR-III-C9-2023-I8 "Chemical host-guest molecular systems for health applications (OMRI for identification of inflammatory pathologies)" contract no. 760283/27.03.2024 funded by European Union – NextGenerationEU.

Citius, Altius, Fortius: New spirocyclic nitroxide spin labels

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New spirocyclic nitroxide spin labels will be presented. The spirocyclic frameworks and their derived spin labels exhibit high stability towards ascorbate reduction and phase memory times which remain excellent with increasing temperature. The spin labels are used to allow DEER measurements on a double cysteine variant of calmodulin at 120 K.

The design philosophy behind the work will be explored, and the experimental results will be examined. The presentation will draw from three recent works by the authors, as well as more recent results.[1-3]

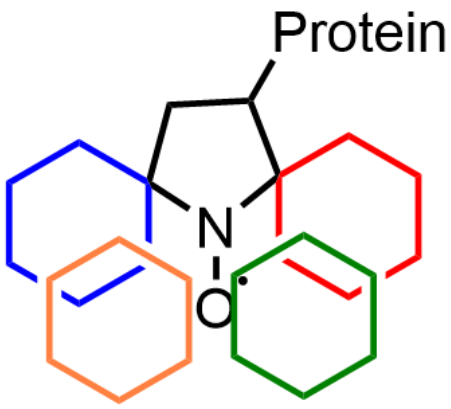

Figure 1: Citius, Altius, Fortius encapsulates our aims for the rational design of new spirocyclic spin labels.

Citius, Altius, Fortius is the original motto of the modern Olympic Games. Translated from the Latin it means Faster, Higher, Stronger. This encapsulates what we are striving for with our new spirocyclic spin labels: they should label quickly and allow for efficient DEER measurement at higher temperatures than tetramethyl nitroxide spin labels, and they should also be resistant (strong) to reduction, perhaps even inside living cells (Fig. 1).

[1] Conformational tuning improves the stability of spirocyclic nitroxides with long paramagnetic relaxation times, Haugland and co-workers, 2023, Commun Chem.
[2] Spirocyclic pyrrolidinyl nitroxides with *exo*-methylene substituents, Haugland and co-workers, 2024, ChemPlusChem.
[3] Sigmatropic rearrangement enables access to a highly stable spirocyclic nitroxide for protein spin labelling, Haugland-Grange and co-workers, 2025, Chemical Communications.

Instrumental effects in optimal control pulse design

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Guinevere Mathies,[2] Ilya Kuprov.[3,1]

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[2] Department of Chemistry, University of Konstanz, Germany;
[3] Dept. of Chemical and Biological Physics, Weizmann Institute of Science, Israel.

Optimal control methods, such as gradient ascent pulse engineering (GRAPE), are used for precise manipulation of spin states. Many of those methods were pioneered in NMR spectroscopy where instrumental distortions are often negligible. However, that is not the case elsewhere: the usual jumble of cables, resonators, modulators, splitters, amplifiers, and filters can and would distort control signals. Those distortions may be non-linear, their inverse functions may be ill-defined and unstable; they may even vary from one day to the next, and across the sample.

In particular, response functions of resonant circuits create ringing artefacts if their input changes rapidly. When physical limits of electromagnetic spectroscopies are explored, this creates two types of problems. Firstly, simulation: the system must be propagated accurately through every response transient, this may be computationally expensive. Secondly, optimal control: circuit response must be taken into account; it may be advantageous to design pulses that are resilient to such distortions. At the root of both problems is the popular piecewise-constant approximation for pulse sequences in the rotating frame; in magnetic resonance it has persisted since the earliest days and has become entrenched in the commercially available hardware.

In this lecture, we report an implementation and benchmarks of recent Lie-group methods that can efficiently simulate and optimise smooth pulse sequences. We also introduce the response-aware GRAPE framework, which accounts for any cascade of differentiable distortions within the optimisation loop, does not require filter function inversion, and produces pulse sequences that are resilient to user-specified distortion cascades with user-specified parameter ensembles.

The framework is implemented into the optimal control module supplied with versions 2.10 and later of the open-source Spinach library; the user needs to provide function handles returning the actions by the distortions and, optionally, parameter ensembles for those actions.

[1] https://doi.org/10.1016/j.jmr.2023.107478
[2] https://doi.org/10.48550/arXiv.2502.02198

Poster Presentations

P1	Jonas **Bach**	Pancake radical p-dimers
P2	Saksham **Mahaja**n	Optimal fabrication of optical-spin defects in van der Waals material for Quantum Sensing
P3	G. **Usevičius**	Superconducting YBCO planar microresonators for conventional high sensitivity ESR
P4	Lorenzo **Catini**	Insights into recombination processes in organic solar cells through electrically detected magnetic resonance
P5	Adam **Brookfield**	EPSRC National Research Facility for EPR Spectroscopy
P6	Maximilian **Mayländer**	EPR characterisation of electrochemically generated and photoinduced charged paramagnetic states in organic semiconductors
P7	Christos **Pliotas**	BioEmPiRe for structural biological EPR spectroscopy; Accessing uncharted ensembles of integral membrane proteins
P8	Jean-Baptiste **Verstraete**	Best averaging practices for summing CPMG echoes
P9	Angeliki **Chatziathanasiou**	Evaluating the binding of inhibitors in the quinone binding site of photosynthetic complex I
P10	Austin **Gamble Jarvi**	Increasing Accessibility and Throughput with an Automated, Multisampling EPR Spectrometer
P11	Gabriel **Moise**	The spin polarised photoexcited quartet state of a copper(II) porphyrin
P12	Katja **Raue**	EPR investigation on the effect of oxygen vacancies on the magnetic and structural properties of mixed Fe-Co perovskites
P13	Nino **Wili**	Pulse EPR is too expensive. Why not build your own spectrometer?
P14	Jonathon **Clark**	Investigating Key Radical Intermediates in Rhenium Based Photocatalytic CO_2 Reduction
P15	Vidmantas **Kalendra**	Pushing the sensitivity boundaries of X-band EPR cryoprobe using a fast microwave switch
P16	William **Myers**	Well-preserved? A *post-crystallo* retrospective of formaldehyde coordination in [FeFe] hydrogenase by frozen solution EPR
P17	Ciarán **Rogers**	High sensitivity pulse EPR using superconducting micro- resonators: applications to volume-limited (bio)molecules in the good and bad cavity limit
P18	Joshua **Wort**	Characterising non-covalent spin probe modulators for human TRPC5 ion channel labelling by EPR spectroscopy
P19	Alberto **Collauto**	PEPR – A pulse EPR facility at Imperial College London
P20	Alberto **Collauto**	'Fast-scan' CW-EPR measurements to enable faster scan rates in *operando* film electrochemical-EPR (FE-EPR) experiments
P21	Jennifer **Naughton**	Structural characterisation of proteins via non-canonical amino acids, a new Gd^{3+} spin label, and Double Electron-Electron Resonance (DEER) Spectroscopy
P22	Calysta **Tesiman**	Chiral Diradicals for Quantum Technologies: Spin-Optical Control in a Trityl–Binaphthalene System
P23	Spartak **Khutsishvili**	Stimulation of stress resistance an antioxidant activity of bionanocomposites based on sulfated polysaccharides with manganese (hydr)oxide nanoparticles
P24	Xinyu **Liu**	Monitoring tension-sensitive states of integral membrane proteins by EPR spectroscopy
P25	Maxim **Neuberger**	CIDEP on a Porphycene-TEMPO system probed via transient EPR
P26	Jacopo **Toninato**	Characterization of peroxy radicals in irradiated PTFE of industrial origin by means of EPR spectroscopy

Pancake radical π-dimers

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Pancake bonding refers to the exceptionally short, co-facial association of two open-shell π-systems, in which extensive SOMO overlap induces a partially covalent character to the contact. Pancake-bonded aggregates have been proposed as molecular components in conducting functional organic materials. To this date, *in silico* studies far outweigh experimental (spectroscopic) investigations and experimental studies are limited to very low temperatures. [1,2]

We present a systematic spectroscopic investigation of Ph-DTDA radicals, [1] which exhibit pancake bonding upon cooling with liquid nitrogen, as suggested by EPR and UV-Vis spectroscopy. These radicals were used as a reference system, alongside covalently bridged derivatives designed to pre-organise the interacting planes, thereby lowering the temperature at which pancake bonding can be observed.

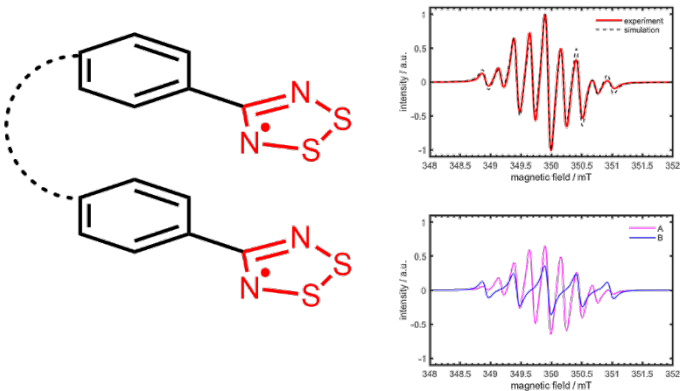

Figure 1. Left: Orientation and overlap of two bridged Ph-DTDA radicals. Right: Experimental and simulated EPR spectrum of the bridged DTDA compounds. The spectrum consists of two subsystems, A and B. Species B shows hyperfine coupling (7 MHz) to two ^{14}N nuclei, resulting in a 5-line spectrum. Species A shows hyperfine coupling (14 MHz) to four ^{14}N nuclei, resulting in a 9-line spectrum.

Redox-innocent linkers of graded length and conformational rigidity were introduced to modulate and control intramolecular overlap. Figure 1 shows the concept of such a linked system. In solution, a spectrum containing two species, A and B is observed. Species B shows hyperfine coupling (7 MHz) to two ^{14}N nuclei, resulting in a 5-line spectrum. Species A shows hyperfine coupling (14 MHz) to four ^{14}N nuclei, resulting in a 9-line spectrum. This observation is attributed to possible exchange coupling between the two radicals - similar to results observed for TOTAPOL, a linked TEMPO biradical. [3]

[1] Review: K. E. Preuss: PANCAKE BONDS: Π-STACKED DIMERS OF ORGANIC AND LIGHT-ATOM RADICALS *Polyhedron* **2014**, *79*, 1.

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Optimal fabrication of optical-spin defects in van der Waals material for Quantum Sensing

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Optically active spin defects in solid state systems have emerged as promising nanoscale quantum sensors due to their atomic size, measurable quantum states and potential for commercial applications. Achieving high sensitivity requires surface proximity of the sensor making atomic defects in van der Waals materials more suitable than 3D-based systems (such as NV centers in diamond). Among these, the negatively charged boron vacancy center (V_b^-) in hexagonal boron nitride (hBN) stands out due to its optically addressable spin states and the measurable response of its spin Hamiltonian to external physical quantities [1]. However, achieving long quantum coherence and stable operation of V_b^- centers in hBN nanoflakes remains a significant challenge. Additionally, the fabrication process is highly invasive for the hBN lattice and often degrades the optical-spin properties of resulting V_b^- centers.

In this study, we successfully fabricated the V_b^- centers in hBN nanoflakes using focused ion beam (FIB) implantation of helium ions (He^+, 25 keV) at varying ion fluence (10^{12} – 10^{15} ions/cm^2) and monitored the effect of defect density on their quantum coherence (Hahn echo T_2 and spin lattice relaxation time (T_1)) and material properties of host lattice. The material changes under different fabrication conditions were measured using Raman spectroscopy. Magnetic sensitivity was also evaluated across different ion fluences (Fig. 1(b)). We identified that beyond a threshold ion fluence (>10^{14} ions/cm^2), the optical-spin properties of V_b^- centers degrade along with the deterioration of the hBN lattice. This indicates a damage threshold concentration of V_b defects in hBN beyond which extended defects start to accumulate and modify the local electric and magnetic field environment of stable V_b^- centers. Therefore, the maximum η_{AC} was achieved for the 10^{14} ions/cm^2. These results are important for practical nanoscale quantum sensing using V_b^- - hBN system.

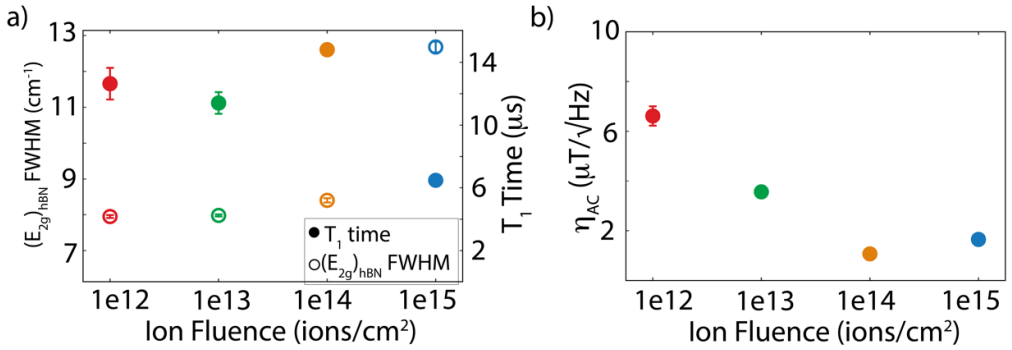

Fig1: a) Results for Raman E_{2g} mode FWHM for flakes with different ion fluence (to study the extent of lattice damage) and the measured spin lattice relaxation times b) Calculated AC sensitivity values of different flakes with varying ion fluence.

[1] Gottscholl *et al.*, Nat. Commun. **12**, 4480 (2021)

Superconducting YBCO planar microresonators for conventional high sensitivity ESR

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Electron spin resonance (ESR) is a powerful spectroscopic technique with applications covering structural biology [1], spin-based quantum technologies [2,3], solid-state physics [4], and other important fields [5]. Despite its versatility, the relatively low sensitivity of conventional ESR poses a significant challenge for studying volume-limited systems, as standard ESR resonators often require samples of microliter volume to achieve detectable spin signals (13). To overcome these limitations, considerable effort has been directed toward the development of planar microwave microresonators of various designs.

Here, we introduce a yttrium barium copper oxide (YBCO) microresonator design (Fig. 1A) along with a simple approach to microresonator coupling via a standard 3D ESR resonator, which together offer the advantages of high-spin number sensitivity with the ability to be readily deployed within any typical ESR laboratory. The microresonator features a spiral geometry designed for X-band (9.5 GHz) ESR with a mode volume of about 7 nL, which provides a 1,000 fold increase in spin number sensitivity over a traditional 3D resonator.

Fig. 1: (A) Fabricated planar YBCO spiral microwave microresonator.

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Insights into recombination processes in organic solar cells through electrically detected magnetic resonance

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The discovery of the Y series of non-fullerene acceptors significantly increased the efficiency of Organic Solar Cells (OSCs), recently surpassing the 20% threshold. The active layer of these devices consists of a blend of organic electron donor and acceptor molecules. Following photoinduced charge separation, spin-dependent charge transport and recombination processes determine the OSC performance. Therefore, a good understanding of these processes is key to further improving device efficiency.

Electrically Detected Magnetic Resonance (EDMR) spectroscopy is a powerful technique for the investigation of spin-dependent processes, as it allows detection of changes in current flowing through fully working, miniaturized devices as a result of microwave-induced transitions. Only spins directly involved in current generation are detected, making this technique exceptionally suited to investigate OSCs.[1]

In this work, two blends with non-fullerene acceptors (PM6:Y6 and PBDB-T:ITIC) and their corresponding fullerene counterparts (PM6:PCBM and PBDB-T:PCBM) were investigated at cryogenic temperatures using pulse EDMR. Rabi nutation experiments were used to investigate the nature of the dominant spin-dependent processes determining the EDMR signal. In all blends except for PM6:PCBM, the presence of spin locking signals in regions of spectral overlap of donor and acceptor revealed contributions from bipolar recombination.[2] The observation of triplet signatures further suggests an additional recombination process involving polarons and triplet excitons.

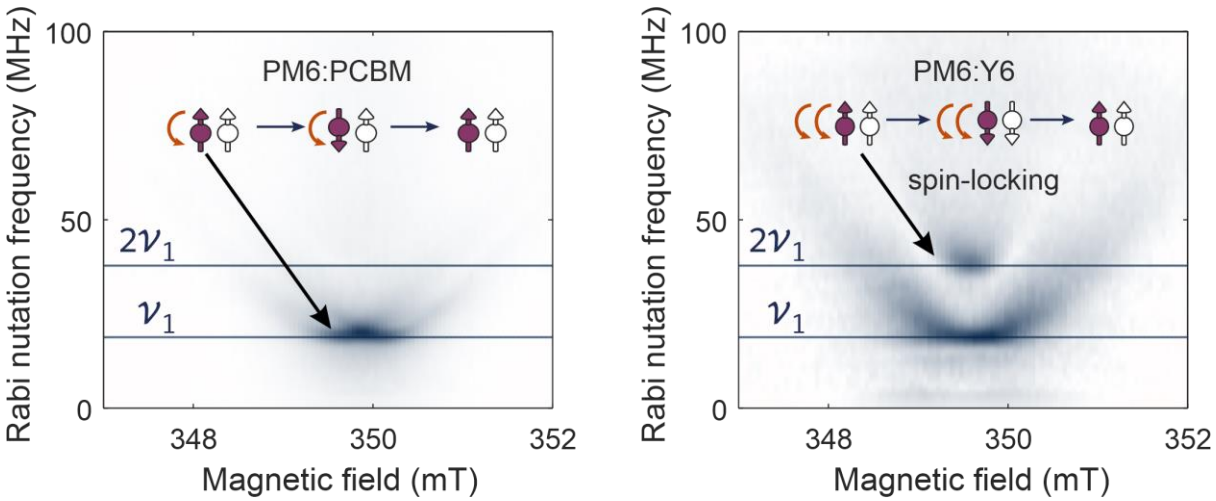

Figure 1: Fourier-transform of a Rabi nutation experiment showing the nutation frequency derived from oscillations of the time-integrated device current ΔI for increasing microwave pulse lengths as a function of static magnetic field for PM6:PCBM (left) and PM6:Y6 (right) OSCs.

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EPSRC National Research Facility for EPR Spectroscopy

Dr Floriana Tuna, Mr Adam Brookfield, Dr Muralidharan Shanmugam, Dr Alice M. Bowen, Prof. David Collison and Prof. Eric J. L. McInnes

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The University of Manchester hosts the EPSRC National Research Facility (NRF) for EPR Spectroscopy, with capabilities for CW (L-, S-, X-, K- and Q-band) and pulsed (S-, X- and Q-band) EPR measurements, electrochemical EPR and optical excitation, along with a Quantum Design MPMS3 SQUID magnetometer (DC, VSM, AC, sample rotation, optical access, ultra-low field and furnace (1000 K) modes). Pulse measurements with a 1 GHz detection bandwidth and a 300 W Q-band amplifier are available. Optical excitation spans the range from 210-2400 nm *via* tuneable OPO lasers, LEDs/broadband, and simultaneous two-wavelength experiments are possible.

Support: The Facility can provide support for most experimental EPR techniques at multi-frequencies and variable temperatures; (1.6 K to 600 K typical, 1000 K at X band) with cryogen-free cryostats. Pulsed hyperfine expertise supports users in accessing ESEEM, ENDOR, EDNMR and HYSCORE methods. Pulsed Dipolar Spectroscopy (PDS) methods including DEER/PELDOR, RIDME, CIDME, and Light induced methods are all supported. Advice about spectrum simulation and access to data modelling software is available. Rapid-Scan capability and a loanable benchtop spectrometer with variable temperature and auto-sampling has recently been implemented.

Updates: New capabilities for 2025 will include a second Q band pulse bridge with 300 W amplification, the addition of L-band pulse; a second bench-top X-band spectrometer with transient output; multi-harmonic detection and an expansion of our complementary UV-vis and electrochemical tools. There has also been heavy investment in custom ENDOR X/Q resonators and matching RF amplifiers.

Access: The EPR NRF welcomes visitors with their samples and provides hands-on training. Samples can be received by post, with sensitive samples being sent in our dry shippers. If you are **preparing a research proposal** for a project that may require access to the Facility, want to undertake a **pilot project** or need to **respond to reviewers**, or just want to **find out how EPR can assist your project**,
please contact us for advice.

EPR characterisation of electrochemically generated and photoinduced charged paramagnetic states in organic semiconductors

Maximilian Mayländer, Marco Ladwig, Niall Curwen, Claudia Tait.

Department of Chemistry, University of Oxford, Oxford, UK.

Charged paramagnetic states in organic semiconductors play a fundamental role in organic electronic devices, including organic solar cells as well as organic electrochemical transistors. A deeper understanding of the charge and spin density distribution in these states can help establish structure–property relationships that are key to improving device efficiencies. EPR spectroelectrochemistry is a powerful tool for the investigation of paramagnetic states of organic donor and acceptor molecules in various chemical environments, such as frozen solution and thin films. By combining hyperfine spectroscopy with DFT calculations, we gain insights into how molecular structure and environment influence electronic properties. In the context of organic solar cells, comparison of isolated charged states in pure materials with the corresponding photoinduced states generated in donor:acceptor blends can then, for example, provide insights into the role of charge delocalization in promoting increased energy conversion efficiency.[1]

We electrochemically generate the charged paramagnetic states of organic donor (e.g., PTB7-Th) and acceptor (e.g., EH-IDTBR) molecules in an adapted spectroelectrochemical cell within an EPR tube,[2] and characterize them by in-situ UV–vis and cw EPR spectroelectrochemistry. The spin density distributions are investigated in greater detail using a series of hyperfine spectroscopic techniques (Q-band ^{1}H Davies ENDOR and ^{14}N ESEEM and HYSCORE). Comparison of the results with measurements on photoexcited donor: acceptor blends revealed differences in spin density distributions attributed to a pronounced dependence of spin delocalization on the molecular environment.

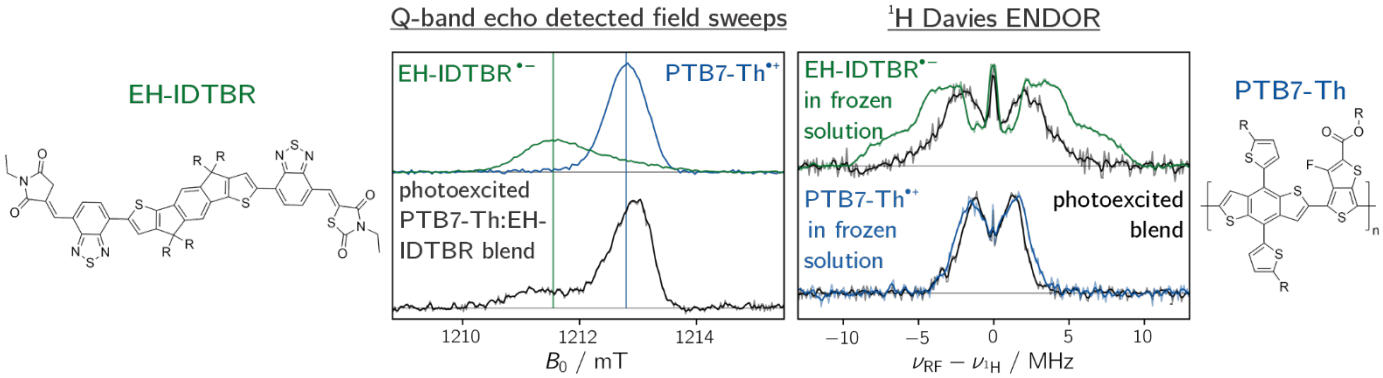

Figure 1. Molecular structures of the acceptor molecule EH-IDTBR and the donor polymer PTB7-Th and comparison of echo-detected field sweeps and Davies ENDOR spectra of the EH-IDTBR anion and PTB7-Th cation with the photoexcited PTB7-Th:EH-IDTBR blend.

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BioEmPiRe for structural biological EPR spectroscopy; Accessing uncharted ensembles of integral membrane proteins

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[1]BioEmPiRe Centre for Structural Biological EPR Spectroscopy, School of Biological Sciences, The University of Manchester, Manchester, M13 9PT, UK

The BioEmPiRe Centre for Structural Biological EPR Spectroscopy in the School of Biological Sciences, at the University of Manchester is an initiative designed to address challenging biological questions using EPR spectroscopy. To date we have addressed key questions in a wide variety of membrane proteins (Fig.1), such as mechanosensitive channels[1], ion pumps[2], ABC-secondary transporters[3], outer membrane proteins[4], human potassium[5], and transient receptor potential channels[6]. We monitored ensembles under membrane tension[1], asymmetries within complexes[2], probed pH dependent regulation[3], accessed uncharted folding landscapes[5], using in-cell EPR[4] and non-covalent spin labelling approaches[6-7].

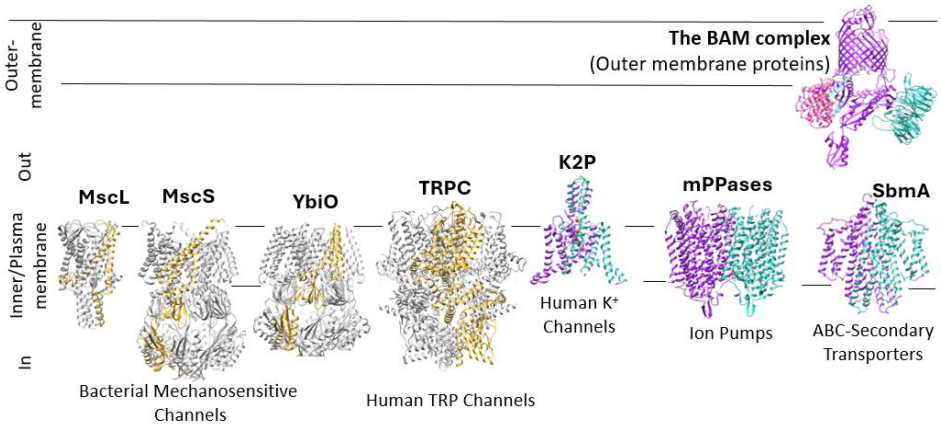

Figure 1: Integral membrane proteins studied by the BioEmPiRe initiative spanning from bacteria to humans and different classes, such as transporters, channels and pumps

BioEmPiRe is equipped with a 300W TWT Bruker pulsed Q-band Elexsys E580 EPR spectrometer, with AWG and integrated Cryogenics He-free system and a benchtop Bruker X-band CW-EPR spectrometer with temperature controller. BioEmPiRe is integrated as a fully equipped wet-laboratory for the preparation of challenging protein samples with research expertise provided by the Pliotas Lab including: cloning, expression, purification, spin labelling and lipid reconstitution from bacterial to complex human proteins. This unique set up provides a complete pipeline from sample preparation to DEER measurements on-site.

[1] Lane^, BJ, Ma^, Y, et al., Bode, BE, Pliotas*, C. (**2024**) ***Structure*** 32: 1-12
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[4] Haysom, SF, Ma, Y, et al., Radford*, SE, and Pliotas*, C. (**2023**) ***Angew Chem Int Ed***, 62, e202218783
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Best averaging practices for summing CPMG echoes

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[1] London Centre for Nanotechnology, University College London, London WC1H 0AH, United Kingdom

The Carr-Purcell-Meiboom-Gill (CPMG) sequence is commonly used across magnetic resonance applications to create a train of echoes (see Figure 1a). Such echoes can be summed to increase the Signal to Noise Ratio (SNR) of an experiment in a process referred to as CPMG averaging. In early work on CPMG averaging in EPR spectroscopy [1, 2], this was done via a simple sum of the echoes. However, the signal intensity decays during the sequence, creating echoes with different SNR which are better summed with weights proportional to said SNRs. Although some exceptions can be found [3], most CPMG averaging data is processed without weights.

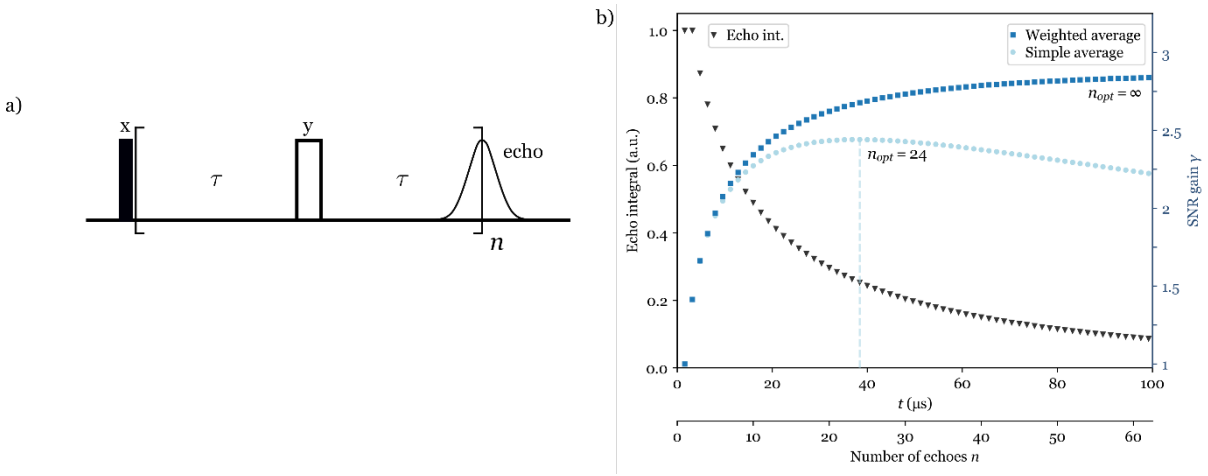

Figure 1: a) Scheme of CPMG sequence. b) Simulated example of integral values from CPMG sequence and associated SNR gain from each averaging method.

This poster presents a detailed analysis of the averaging methods, showing that SNR gains of 10-20% (20-40% of measurement time) are achievable thanks to the basic step of adding weights (see Figure 1b). To further optimise the sequence, analysis of the optimum echo integration strategy is presented. A formula is proposed for the optimal choice of interpulse delay when echoes are longer than the dead time and refocusing pulse duration.

[1] Twig, Y., Dikarov, E., Hutchison, W. D. & Blank, A. Note: High sensitivity pulsed electron spin resonance spectroscopy with induction detection. *Review of Scientific Instruments* **82** (2011).
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Evaluating the binding of inhibitors in the quinone binding site of photosynthetic complex I

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[2] Department of Life Sciences, Sir Ernst Chain Building-Wolfson Laboratories, Imperial College London, South Kensington Campus, London, SW7 2AZ, United Kingdom;
[3] Syngenta Ltd., Jealott's Hill Research Centre, Bracknell, RG426EY, United Kingdom.

The quinone-binding sites of photosystem II are common herbicide targets across the photosynthetic electron transport chain (PETC) [1], due to their association with important cellular processes, such as ATP production and carbon fixation [2]. In this study, we have used EPR in combination with biochemical and computational tools to understand the inhibition of a novel, promising target, photosynthetic complex I (PS-CI), ultimately aiming to improve agricultural sustainability.

We report our progress in the development of an activity assay to observe the complex's activity in solution as well as in a native-like environment for the first time (Figure 1b).

We further investigate the interactions between the quinone-binding site of PS-CI and potential inhibitors, exploiting our knowledge of PS-CI's homolog, respiratory complex I (R-CI) [3]. CW-EPR measurements indicated that certain R-CI inhibitors can inhibit the Q-site of PS-CI. Furthermore, a combination of computational studies and pulsed EPR techniques proved that, at least in the case of some inhibitors, the Q-site inhibition isn't caused by direct interactions with the Fe-S clusters of PS-CI.

These observations are valuable in order to rationally design a new generation of herbicides.

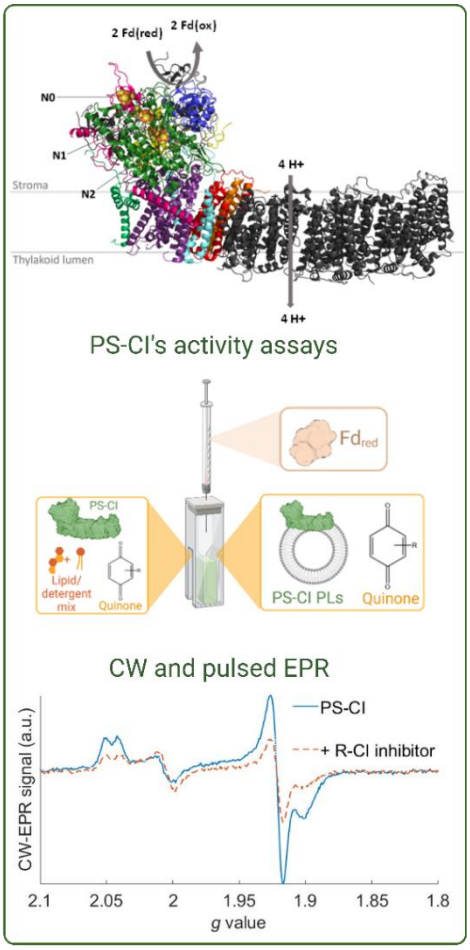

Figure 1: (a) Structure of *T. elongatus* PS-CI (Photosynthetic complex I) (PDB: 6HUM). (b) Representation of activity assays. (c) CW EPR spectra of isolated PS-CI in the absence and presence of a R-CI's inhibitor.

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Increasing Accessibility and Throughput with an Automated, Multisampling EPR Spectrometer

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Pulsed Dipolar Spectroscopy (PDS), a branch of Electron Paramagnetic Resonance (EPR) spectroscopy focused on the measurement of nanoscale electron-electron distances via the strength of their dipolar interaction, has garnered significant interest within the scientific community in recent decades. PDS can provide rich structural and dynamic information on biomolecules that may be difficult or impossible to attain through alternative biophysical methods such as Cryo-EM, NMR, and X-ray crystallography, making it an attractive technique in the field of structural biology at large. However, PDS faces obstacles to its widespread adoption into standard structural biology workflows, such as the steep learning curve to conducting distance measurements and low sample throughput. Here, we present a commercial EPR system designed around mitigating these limiting factors.

The system presented is based around a compact superconducting resonator device, enabling high stability and micromolar sensitivity with small sample volumes and a compact form factor. These properties allow for multisample capabilities, with up to five samples being introduced into the cryostat simultaneously. As well, the stability and sensitivity of the instrument allow for long, uninterrupted data collection with no phase drift, for unattended sequential acquisitions. These advancements are further facilitated by the automation of sample handling, sample characterization, PDS data collection, and distance analysis requiring minimal user input. The system presented here represents important progress in broadening the accessibility and application of EPR into diverse scientific disciplines.

The spin polarised photoexcited quartet state of a copper(II) porphyrin

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Spin polarised excited states are attractive for applications in molecular spintronics where an essential requirement is the ability to inject spin polarised currents into molecular systems. Furthermore, high-spin complexes are desirable as qudits because their spatially compact but expanded Hilbert space can be exploited, for example, in quantum error correction algorithms. In this context, initialisation of spin qudits by photoexcitation is advantageous because it often leads to highly spin polarised states (pure states) as opposed to thermalised states. In light of these promising applications, understanding the properties of quartet states (S=3/2) generated by photoexcitation of a ground doublet state (S=1/2) is regarded as an important step forward (see ref. [1] for a comprehensive review).

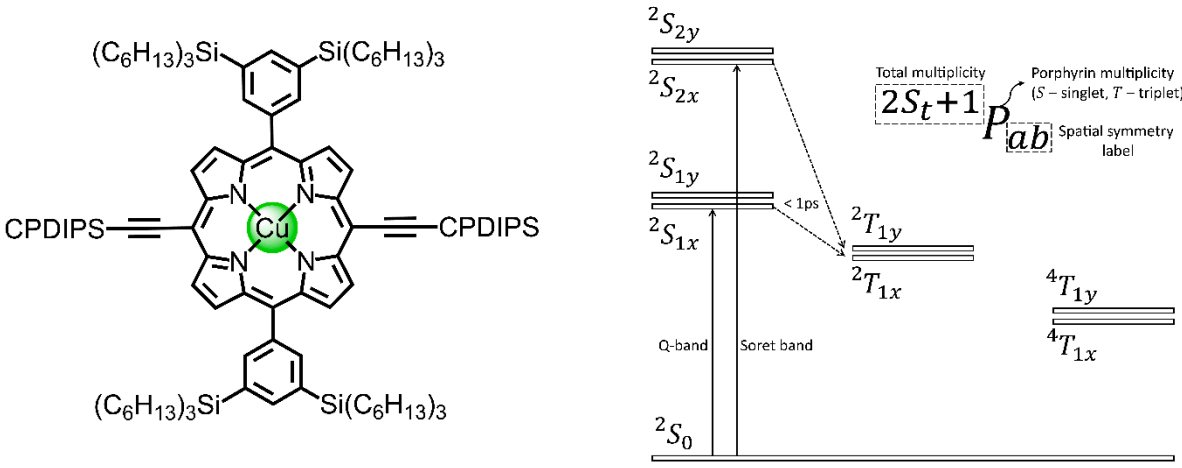

Figure 1. (Left) Structure of the copper(II) porphyrin investigated here. (Right) Simplified Jablonski diagram for copper(II) porphyrins.

This work concerns the investigation of the photophysical and magnetic properties (g-factors and zero-field splittings) of the photoexcited quartet state of a copper(II) porphyrin. The nanosecond photophysics of the complex is explored using transient absorption spectroscopy, whereas the magnetic parameters and spin polarisation are measured using pulse and transient electron spin resonance. The emergence of spin polarisation is discussed using a toy model which captures the fundamental spin dynamics involved in the formation of the quartet state.

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EPR investigation on the effect of oxygen vacancies on the magnetic and structural properties of mixed Fe-Co perovskites

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[1] Institute of Molecular Physical Science, Department of Chemistry and Applied Life Sciences, ETH Zurich, Vladimir-Prelog-Weg 2, 8093 Zurich, Switzerland;
[2] Department of Mechanical and Process Engineering, ETH Zurich, Leonhardstrasse 21, 8092 Zurich, Switzerland;

Magnetically ordered oxides possess an inherent magnetization due to exchange or superexchange couplings between paramagnetic metal ions. These magnetic properties and the structure of the materials can be modified by introducing oxygen vacancies. In this work, the influence of oxygen vacancies on the magnetic and structural properties of a series of Co and Fe based perovskites are investigated. These materials are of particular interest due to their ability to supply oxygen for the oxidative dehydrogenation of alkanes by forming oxygen vacancies [1].

The investigated series includes the well reported $SrFeO_{3-\delta}$ and $SrCoO_{3-\delta}$ and the newly synthesised $SrFe_{0.6}Co_{0.4}O_{3-\delta}$ and $SrFe_{0.2}Co_{0.8}O_{3-\delta}$. The materials were reduced by a thermal treatment under inert conditions, leading to the formation of oxygen vacancies, while simultaneously monitoring the transformation in-situ by CW X-band EPR spectroscopy and EPR-detected conductivity (Fig. 1). Ex-situ CW X-band EPR spectroscopy temperature series (298 K - 10 K) measurements were performed for the as-synthesised and the reduced materials. For $SrFeO_{3-\delta}$ and $SrCoO_{3-\delta}$ the Curie-Weiss analysis agrees with literature reports (Fig. 2) [2]. For $SrFe_{0.6}Co_{0.4}O_{3-\delta}$ and $SrFe_{0.2}Co_{0.8}O_{3-\delta}$ magnetic phase transitions were detected and hypothesis for the structures of the as-synthesised and the reduced materials are proposed.

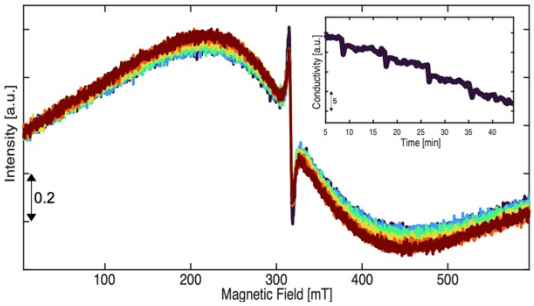

Fig. 1 In-situ CW EPR and conductivity measurements for the as-synthesised $SrFeO3_{3-\delta}$ during the reduction.

Based on these results, we interpret the magnetic behaviour of the materials by expanding the Goodenough and Kanamori rules [3] to non-ideal, non-octahedral metal ions and non-linear M-O-M superexchange systems. This work will be useful for future investigation of the magnetic and conductivity properties of magnetically ordered oxides.

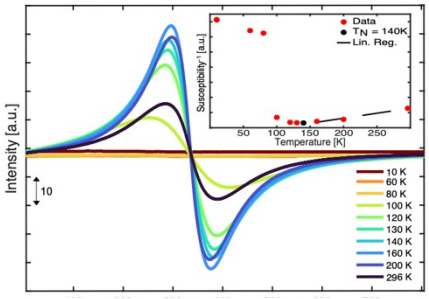

Fig. 2 Ex-situ CW EPR temperature series and the Curie-Weiss analysis for the as-synthesised $SrFeO3_{3-\delta}$.

[1] G. Luongo, et.al., *Phys. Chem. Chem. Phys.* **2020**, 22, 9272-9282
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Pulse EPR is too expensive. Why not build your own spectrometer?

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[2] Institute of Molecular Physical Sciences, ETH Zurich, Switzerland.
[3] Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland.

A complete commercial high-power X/Q-band EPR spectrometer costs about 1.5 Mio € [1]. For comparison, with this money a university could buy about four 400 MHz NMR spectrometers, two 600 MHz, or one subscription to Elsevier journals for about a year.

While commercial, full-package solutions certainly have their place in scientific research, we are of the opinion that in many cases home-built solutions are more attractive, due to a few reasons: **1)** Lower costs. **2)** Better quality of mw mixing and AWG control. **3**) The most widespread EPR spectrometer control software is outdated. **4)** Troubleshooting and replacing a defective component is much faster **5)** Flexibility. It's much easier to implement new hardware or software ideas.

After A. Doll first constructed a pulse EPR bridge fully controlled by a fast arbitrary waveform generator (AWG) at ETH Zurich around 2014, we **1)** replaced a dying commercial X-band console with a home-built X/Q-band EPR & ENDOR spectrometer with initial automation (D. Klose) **2)** constructed a new X-band EPR/DNP spectrometer with home-built bridge and a commercial magnet and cryostat at Aarhus University (Denmark) (N. Wili), and **3**) are finishing up an automatable Ka-band spectrometer with a more cost-effective, less-powerful AWG and a solid-state power amplifier (H. Karas).

This poster will show some pictures and data of these spectrometers, but mostly it should act as a meeting point for researchers who would be interested in getting help to build their own pulse EPR spectrometer. No special electrical engineering knowledge is needed if an existing design is copied.

We are happy to share experiences (incl. prices), parts lists, software, and advice. Our support would usually be informal, but we are thinking of developing a more formal consulting solution as well.

[1] https://ted.europa.eu/en/notice/-/detail/274160-2022 (Note the typo, 11’200’000 € should hopefully be 11’200’000 DKK.)

Investigating Key Radical Intermediates in Rhenium Based Photocatalytic CO_2 Reduction

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CO_2 is one of the most potent molecules contributing to anthropological global warming and improving methods for the removal of CO_2 from the atmosphere are of great interest. [1] Here, molecular photocatalysts have attracted great attention due to their ability to generate high energy intermediates, which can then be used as precursors for regenerating fuel or building blocks for petrochemicals, whilst removing harmful CO_2 from the atmosphere. [2] Rhenium(I) tricarbonyl polypyridyl derivatives, $Re(CO)_3(NN)X$, where X = Cl, Br, CN, SCN, offer some of the highest selectivity and quantum efficiencies for molecular photocatalysts.

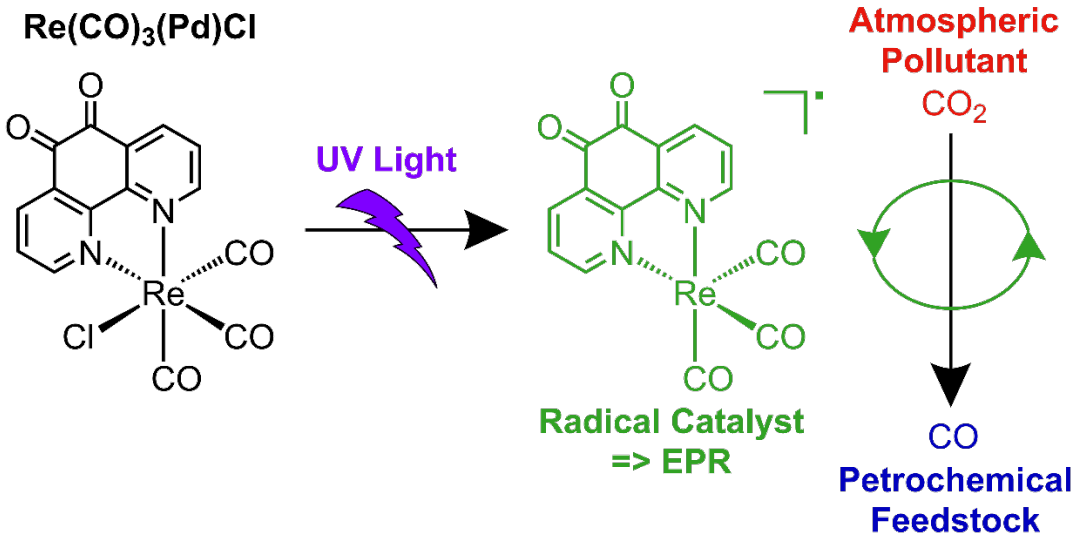

Figure 1:The proposed mechanism for generating the active catalyst in the reduction of CO_2 to CO. Photolysis of $Re(CO)_3(Pd)Cl$ (left), by UV light, leads to formation of a radical based Re species which is proposed to be the active catalyst in the photoreduction of CO_2.

One such rhenium based compound is $Re(CO)_3(Pd)Cl$, Figure 1 (left), which has been shown to photocatalyse the production of CO, an important feedstock for numerous industrial processes, from the reduction of CO_2. [3] The mechanism proposed, Figure 1 (right), involves generating a radical based intermediate which we aimed to characterise with EPR spectroscopy. By using a combination of cwEPR, time resolved EPR (trEPR), and hyperfine spectroscopy, this radical intermediate, from the photolysis of $Re(CO)_3(Pd)Cl$, could be studied.

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Pushing the sensitivity boundaries of X-band EPR cryoprobe using a fast microwave switch

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We present a new design of an X-band EPR cryoprobe based on a fast microwave switch and a cryogenic low-noise microwave amplifier that are placed close to the sample in the same cryostat [1]. The probehead supports high-power (100 W) pulsed EPR experiments and is compatible with standard EPR resonators and samples. In contrast to the directional coupler design of the EPR cryoprobe reported previously, the fast microwave switch fully isolates the microwave amplifier from input thermal noise without microwave power suppression allowing us to approach the sensitivity limit of cryoprobes for pulsed EPR experiments. We benchmark the performance of our cryoprobe setup against a standard commercial EPR instrument revealing a significant sensitivity improvement, which reduces the measurement time by a factor of about 250× at 6 K sample temperature. We also show that the sensitivity of our new X-band cryoprobe design matches that of a standard Q-band setup for double electron–electron resonance experiments.

Acknowledgments. The research was supported by funding from the European Union HORIZON-MSCA-2021-PF-01 Marie Sklodowska-Curie Fellowship (Project ID:101064200) and the Research Council of Lithuania (LMTLT), agreement No. S-LLT-23-1.

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Well-preserved? A *post-crystallo* retrospective of formaldehyde coordination in [FeFe] hydrogenase by frozen solution EPR.

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As a strong electrophile, formaldehyde (HCHO) is known to bind rapidly and reversibly to [FeFe] hydrogenase, inhibiting hydrogen production whilst bound. Understanding why and how this happens is essential to industrial applications of hydrogenase, or a hydrogenase mimic, as a catalyst to interconvert methanol and formaldehyde. Binding occurs when a highly reactive metal-hydrido species is formed within the catalytic cycle. As this highly-reduced state of the cluster is EPR-active, a range of isotopic labelling and pulsed EPR methodology is possible. EPR was used to observe a range of binding mode(s) of formaldehyde in *Chlamydomonas reinhardtii* [FeFe]-hydrogenase [1]. The standard pulsed EPR techniques including electron−nuclear double resonance spectroscopy and HYSCORE with auxiliary ^{2}H-ESEEM confirm that a multi-component, complex distribution of formaldehyde has limitations on the distribution of the molecule in the vicinity of the H-cluster. While an Fe-bound formaldehyde was thought to be a metal-hydrido mimic, more recent crystallographic work observes an entirely different binding mode via the bridging secondary amine, but nonetheless inhibiting the proton transfer capability of the cluster [2]. One may conclude therefore that nucleophilicity of amines act as a competitive coordinator, affording methylol and Schiff base derivatives of amines {asparagine, glutamine, histidine, lysine, and tryptophan} that are characteristic in formaldehyde-based protein cross-linking methodology, seen here through crystallographic characterisation not only of the bridging H-cluster amine, but also in lysine groups. Given the new information of [FeFe]-hydrogenase protein crystals modified with formaldehyde, the prior work of dipolar-couplings used in frozen solution EPR is reconsidered, where preparation difference *in solution* may lead to other proximal amine derivatives as potential loci of ^{13}C and ^{2}H signals.

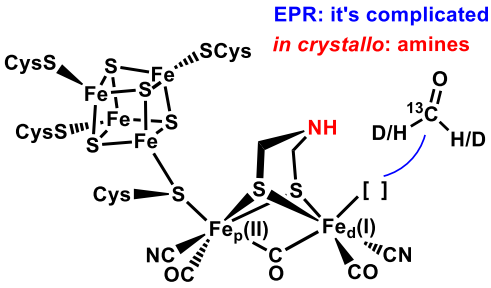

Figure 1: Structure of the H-cluster of [FeFe] hydrogenase

[1] Bachmeier A, Esselborn J, Hexter SV, Krämer T, Klein K, Happe T, McGrady JE, Myers WK, Armstrong FA. How formaldehyde inhibits hydrogen evolution by [FeFe]-hydrogenases: determination by 13C ENDOR of direct Fe–C coordination and order of electron and proton transfers. Journal of the American Chemical Society. 2015 Apr 29;137(16):5381-9.

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High sensitivity pulse EPR using superconducting micro-resonators: applications to volume-limited (bio)molecules in the good and bad cavity limit

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In the pursuit of an optimised workflow for high sensitivity pulse EPR, superconducting planar microresonators have emerged as a versatile and low-cost tool compatible with commercial EPR set-ups.[1] In particular, high temperature yttrium barium copper oxide (YBCO) microresonators, which feature reduced mode volumes and high Q-factors, offer enhanced absolute spin number and spin concentration sensitivities for volume-limited samples, while also enabling large microwave-to-magnetic field conversion factors.[2] Although applications in areas such as spin-based quantum information processing have been reported this typically requires tailored samples, specialised equipment and millikelvin temperatures.[3]

In this work we investigate applications of YBCO microresonators for the measurement of “real” samples using common spin centres (*e.g.* nitroxides, trityl and Fe-S clusters), in scenarios where the spin linewidth, Γ_S, is greater (good-cavity limit) or narrower (bad-cavity limit) than the resonator bandwidth, $\Delta\nu$. We quantify film thickness by different sample preparation methods on the surface of the YBCO microresonator using confocal microscopy, before determining signal-to-noise ratios (SNR) *via* spin echo measurements. Further, we leverage the enhanced sensitivity at the detection spin echo to perform single-frequency pulsed dipolar spectroscopy (PDS) experiments. We determine a three orders of magnitude enhancement in the absolute spin number sensitivity and a reduced sample volume by a factor of 6000, compared to a 3D cavity, with a conversion factor of 95 $G/W^{1/2}$. Working towards robust double-resonance experiments, we present preliminary results featuring a microresonator array localised on a transmission line that has the potential to allow for multi-harmonic detection and ultra-wide bandwidth pulsing in high Q-factor resonators.

We expect these results to lay the foundation for further advancements in high sensitivity pulse EPR using superconducting microresonators, which is expected to have a major impact in areas such as film-electrochemical EPR and structural biology.

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[2] Y. Artzi *et al.*, *J. Mag. Res.* **2022**, *334*, 107102.
[3] Z. Wang *et al.*, *Nature* **2023**, *619*, 276–281.

Characterising non-covalent spin probe modulators for human TRPC5 ion channel labelling by EPR spectroscopy

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Electron paramagnetic resonance (EPR) pulse dipolar spectroscopy (PDS) combined with site-directed spin-labelling (SDSL) has become a powerful tool to elucidate membrane protein structure under near-native conditions.[1] Commonly, cysteine residue handles are introduced and nitroxide radicals are conjugated via sulfhydryl moieties. However, this spin-labelling strategy is problematic in cysteine-rich systems or for cysteines non-permissive to mutagenesis. Indeed, genetic labelling approaches, such as Cu(II)-chelates coordinated by double-histidine motifs,[2,3] offer a viable alternative, but in native proteins relies on serendipity of histidine configuration.

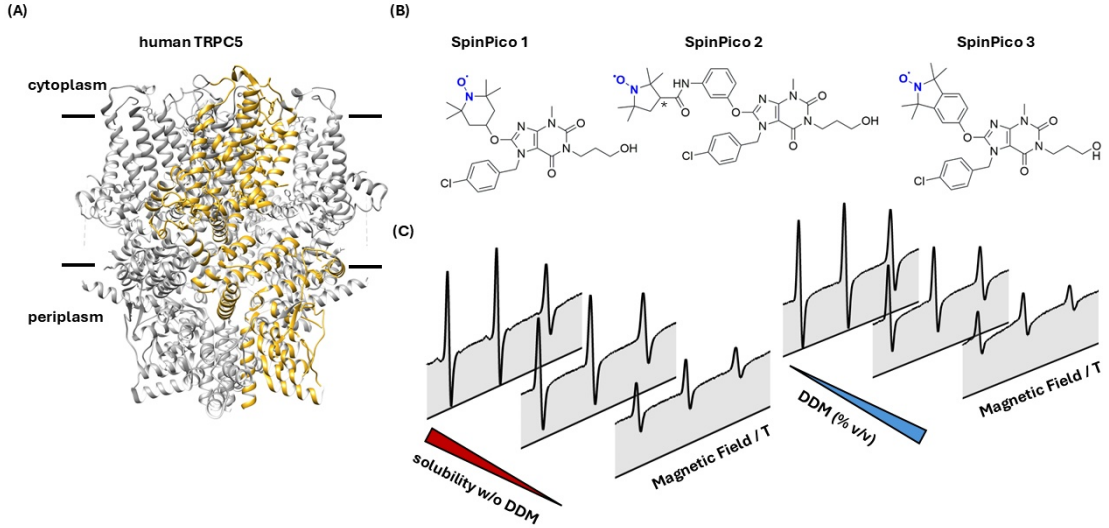

Figure 1: **(A)** Human TRPC5 tetrameric structure, with a single subunit indicated in gold. **(B)** Chemical structures of the three novel nitroxide spin probes: SpinPico1, SpinPico2, and SpinPico3. **(C)** CW-EPR spectra (left) SpinPico probes in absence of DDM, (right) SpinPico3 in presence of varying concentrations of DDM.

Herein we develop and characterise – through CW-EPR, relaxation measurements, and PDS – the utility of high-affinity xanthine-based nitroxide spin probes to study functional states of a candidate therapeutic target: full-length, wildtype human transient receptor potential channel 5 (TRPC5).[4] These bespoke paramagnetic activator and inhibitor analogues may also present a future platform to label other members of the TRPC family.

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PEPR – A pulse EPR facility at Imperial College London

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PEPR, the Centre for Pulse EPR at Imperial College London, is a pulse EPR research facility launched in 2021.

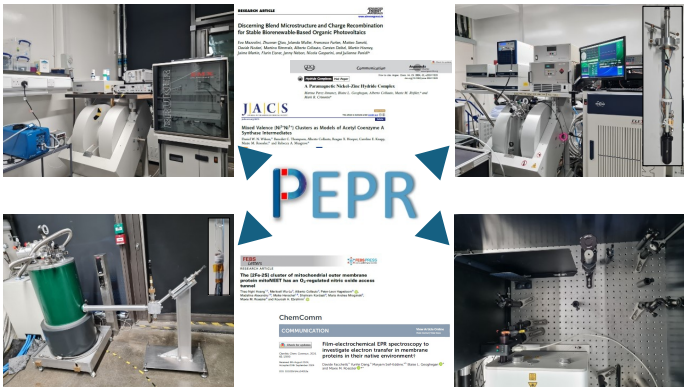

Figure 1: Equipment available at PEPR and some highlights from our publications.

We provide access to state-of-the-art equipment, including (*i*) a Bruker E580 CW- and pulse spectrometer operating at X- and Q-band frequencies with AWG and pulse ENDOR capabilities combined with a pulsed laser (λ = 410-2600 nm, t_p = 6 ns) for sample photoirradiation inside the EPR resonator, as well as (*ii*) a Bruker EMX X-band CW-EPR spectrometer with high-sensitivity resonators for standard EPR detection and a dual-mode cavity for parallel-mode detection.
Temperature control in the 300 K – 2 K range is achieved by means of closed-circuit cryostats (Cryogenic Ltd.), available for both Flexline and waveguide microwave resonators; an additional N_2 variable-temperature unit (Bruker) is available for continuous-wave measurements between 90 K and above room temperature.

Besides commercially available equipment, PEPR has from some unique features:

- A high-sensitivity setup for X-band pulse EPR measurements, compatible with Bruker Flexline resonators, based on a cryogenically cooled preamplifier [1]. This setup can boost the signal-to-noise ratio at low temperatures by a factor of up to 10, resulting in a considerable reduction of the measurement time and thereby enabling measurements on a very small number of spins.
- A spectroelectrochemical setup based on film electrochemistry [2] for the detection of paramagnetic species generated inside the EPR sample tube by applying a potential to the studied system.

Here we will showcase the latest updates on the available equipment and some highlights from research projects that are currently running at PEPR.

[1] M. Šimėnas, J. O'Sullivan, C. W. Zollitsch, O. Kennedy, M. Seif-Eddine, I. Ritsch, M. Hülsmann, M. Qi, A. Godt, M. M. Roessler, G. Jeschke, J. J. L. Morton, *J. Magn. Reson.* **2021**, *322*, 106876.

[2] M. Seif-Eddine, S. J. Cobb, Y. Dang, K. Abdiaziz, M. A. Bajada, E. Reisner, M. M. Roessler, *Nat. Chem.* **2024**, *16*, 1015–1023.

‘Fast-scan’ CW-EPR measurements to enable faster scan rates in *operando* film electrochemical-EPR (FE-EPR) experiments

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Operando film-electrochemical EPR spectroscopy [1] enables the real-time detection of paramagnetic intermediates in electrocatalytic reactions.

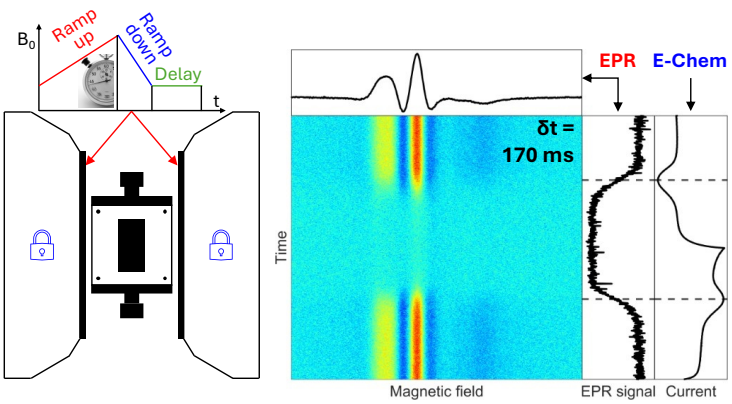

Figure 1: The proposed ‘fast-scan’ acquisition scheme uses the setup scan coils of Bruker EPR spectrometers to sweep the magnetic field. This reduces the acquisition time for CW-EPR scans to ~200 ms, enabling higher scan rates in FE-EPR experiments.

The conventional acquisition protocol is built upon a standard cyclic voltammetry (CV) experiment during which CW-EPR spectra are recorded. This results in a variation of the applied potential during the EPR data acquisition. Currently, the upper limit of the achievable scan rate in the CV experiment is ~15 mV/s, resulting from an acquisition time of ~5 seconds for each CW-EPR spectrum. This limitation prevents the characterisation of fast electron transfer processes, which require faster scan rates.

For fast CW-EPR sweeps only a minor part of the scan time is used for actual data acquisition; a considerable fraction is used by the spectrometer to reinitialise the scan routine. This results in an inefficient acquisition protocol. The use of rapid-scan EPR (RS-EPR) is a possible solution to this issue, however it requires dedicated hardware, not available in most of the EPR laboratories. Alternatively, the acquisition schedule can be reversed by performing time-domain CW-EPR acquisitions during which the potential is changed and repeating this experiment for different magnetic field values. This approach is characterised by an extended time required to sample the entire CW-EPR spectrum and is therefore only practicable if the electrochemical system under investigation is highly stable.

Bruker CW-EPR spectrometers are equipped with setup-scan coils (Figure 1) able to generate rapid (~200 ms, *i.e.* more than an order of magnitude improvement compared to the conventional set-up) field sweeps with a scan width of up to 200 G. In this work we demonstrate that it is possible to use these coils to reduce the impact of the reprogramming time on the acquisition of *operando* electrochemical EPR spectra.

[1] M. Seif-Eddine, S. J. Cobb, Y. Dang, K. Abdiaziz, M. A. Bajada, E. Reisner, M. M. Roessler, *Nat. Chem.* **2024**, *16*, 1015–1023.

Structural characterisation of proteins via non-canonical amino acids, a new Gd^{3+} spin label, and Double Electron-Electron Resonance (DEER) Spectroscopy

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DEER spectroscopy is a valuable technique for elucidating protein structure, dynamics, and function, combining EPR with site-directed spin-labelling to obtain long range distances from dipolar coupling measurements between two electron spins. Spin labels for DEER are typically attached to proteins of interest via prior site-directed mutagenesis of the sequence to incorporate cysteine residues, almost exclusively, for subsequent tagging. This is predominantly done with a nitroxide spin label considered the gold-standard among spin labels, known as MTSL.

However, this chemistry renders proteins containing numerous surface-exposed cysteine amino acid residues incompatible for study through the standard labelling techniques. Currently there is no generally applicable labelling technique not reliant upon cysteine labelling, and to address this limitation, non-canonical amino acids (ncAAs) can be genetically incorporated via amber stop codons for site-specific installation of bio-orthogonal reaction handles within proteins of interest, like ERp29. This endoplasmic reticulum luminal protein functions as a chaperone and is also regarded as a model protein due to its cellular presence and high-quality x-ray structure, rendering it ideal to ascertain viabilities of new techniques for protein study.

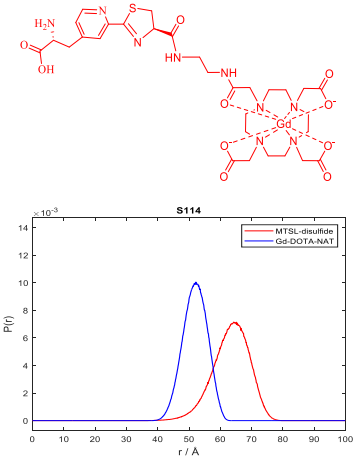

Figure 1: (top) Structure of Gd^{3+}-DOTA spin label conjugated to cyanopyridylalanine via NAT-click reaction. (bottom) Comparisons of distance distributions for Gd^{3+}-DOTA and MTSL labelling of ERp29 at position S114.

This research aims to develop a new generally applicable spin labelling technique for proteins with natively crucial cysteine residues based on the Nitrile-AminoThiol (NAT) chemical click reaction. These reactions enable the conjugation of designed Gd^{3+} tags each containing an aminothiol group to genetically encoded cyanopyridylalanine ncAAs within proteins of interest [1]. Here, we demonstrate the first successful production of double labelled, cysteine-containing ERp29 proteins via NAT-click chemistry, and DEER data displaying a Gd^{3+}-Gd^{3+} distance of approximately 65 Å, as seen in Fig. 1.

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58th International Meeting of the RSC ESR Group, *London, UK*

Chiral Diradicals for Quantum Technologies: Spin-Optical Control in a Trityl–Binaphthalene System

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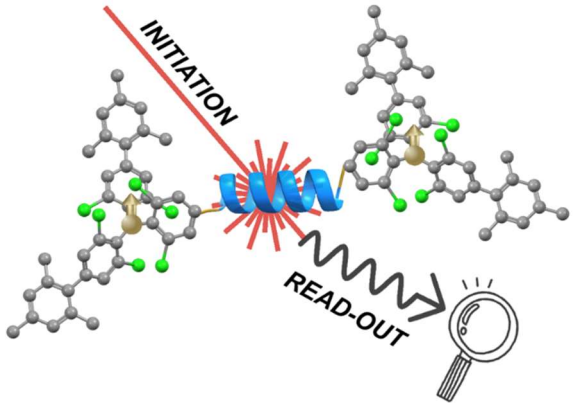

Molecular systems with spin-optical readout and manipulation capabilities offer a novel approach to quantum information transfer [1]. Among these, organic semiconductor radicals are particularly attractive due to their tuneable spin environments, synthetic versatility for precise spin placement, and scalability. However, the relationship between chirality and spin control in diradical systems remains underexplored [2].

Here, we report the emergence of a chiral biradical system comprising two trityl radical units bridged by a chiral binaphthalene moiety, exhibiting a thermally accessible triplet state as revealed by EPR spectroscopy. Temperature-dependent EPR measurements in solution were employed to probe the spin states, while pulsed EPR techniques, including Rabi nutation, enabled the investigation of coherent spin manipulation. Complementary density functional theory (DFT) calculations and EPR simulations supported the experimental findings and provided estimates of spin–spin coupling parameters. The system displays clear EPR signatures characteristic of a triplet state with zero-field splitting. Notably, Rabi nutation experiments revealed asymmetric oscillations, indicative of microwave-driven spin transitions within a thermally populated triplet manifold. Simulations successfully reproduced key spectral features and confirmed substantial dipolar coupling between the two spin centres.

The chiral diradical system exhibits key properties of a promising molecular qubit: a thermally accessible triplet state, and coherent spin dynamics. These results support the emergence of molecular diradical systems as a potential platform for scalable optically addressable quantum technologies.

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Stimulation of stress resistance an antioxidant activity of bionanocomposites based on sulfated polysaccharides with manganese (hydr)oxide nanoparticles

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Some important agricultural plants are very sensitive organisms to various types of stress, including phytopathogen, such as *Clavibacter michiganensis* subsp. *sepedonicus* bacteria (*Cms*). During the study of potato tissues the EPR spectra of plant tissues showed a singlet with a *g*-factor of 2.004(2) and a line width (Δ*H*) 8(1) G. The signal parameters are characteristic of stable semiquinone radicals. The level of semiquinone radicals can serve as an indicator of plant resistance to stress and is determined by the degree of damage to the cell structure, moisture loss, and other processes. To evaluate the stress state of plants under the action of the obtained manganese-containing bionanocomposites (NCs) based on natural polysaccharides (arabinogalactan, ι- and κ-carrageenans), the following biochemical parameters were studied: peroxidase activity, the content of reactive oxygen species (ROS), the amount of lipid peroxidation (LPO) products, diene conjugates (DC) and malonic dialdehyde (MDA) in tissues of roots and leaves. These bioindicators are very sensitive towards various stress factors. Also plants colonized by the pathogen were used to assess the level of stress using ROS. In the case of NCs treatment of plants with *Cms*, a decrease in the ROS content was noted. The obtained result indicates the activation of the protective functions of the plant organism under stress. The obtained results show that NCs have a pronounced antiradical action. Treatment of infected plants with this composite reduced the content of ROS, DC and MDA in tissues, indicating the intensity of destructive processes under the influence of ROS, among which there were radicals. Thus, it can be concluded the available results indicate that NCs improve the protective functions of the plant organism due to an increase in the activity of antioxidant enzymes. Antibacterial and antioxidant activity has been demonstrated on manganese oxide nanoparticles without polymer coating [1, 2].

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Monitoring tension-sensitive states of integral membrane proteins by EPR spectroscopy

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Membrane proteins are vital components of cellular function, mediating processes such as ion transport and signal transduction. Mechanosensitive ion channels can respond to mechanical forces, playing crucial roles in cellular homeostasis. Molecular tools to and methods to probe their highly dynamic states are lacking. In our recent research, we developed new molecular tools to enable tension application in lipid membranes and monitor tension-sensitive states of mechanosensitive channels by double electron-electron resonance (DEER) spectroscopy.[1]

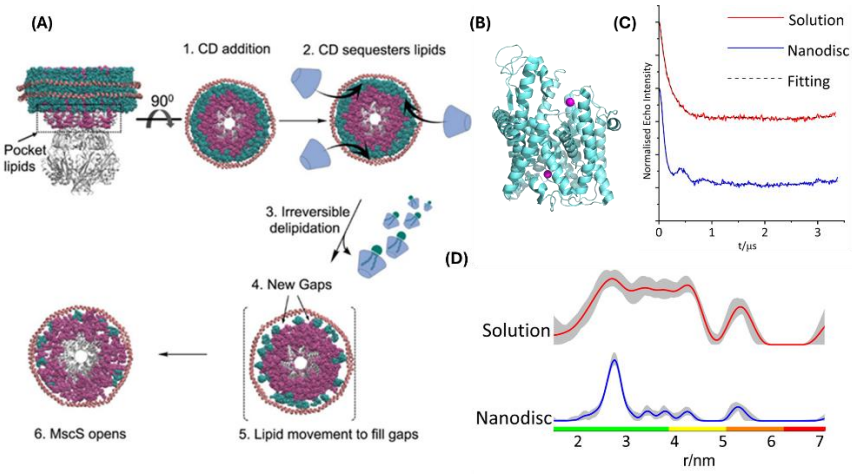

Figure 1. (A) Schematic of cyclodextrin (CD) induced membrane tension and associated conformational changes of MscS.[1] (B) The X-ray structure of SecYEG translocon. Labelling sites are shown in magenta spheres. (C) Background corrected raw data and fitting of PELDOR measurements of SecYEG in two conditions. (D) Distance distributions obtained from DEER experiments. 95% confidence intervals (CI) are shown as shaded regions and traffic light on x-axis indicates the reliability of DEER distribution.

We here combine cyclodextrin-induced tension application in membranes with DEER to investigate candidate mechanosensitive membrane proteins belonging to structurally diverse membrane protein classes, such as the secYEG translocon.[2][3] Preliminary DEER distance measurements indicate that secYEG adopts a distinct, monodisperse conformation in lipid bilayers compared to detergent solution, suggesting that the lipid membrane has an dramatic effect on structure of secYEG. Our method could be applied to distinct classes of integral membrane proteins for identifying and characterising novel tension sensitive states by DEER.

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CIDEP on a Porphycene-TEMPO system probed via transient EPR

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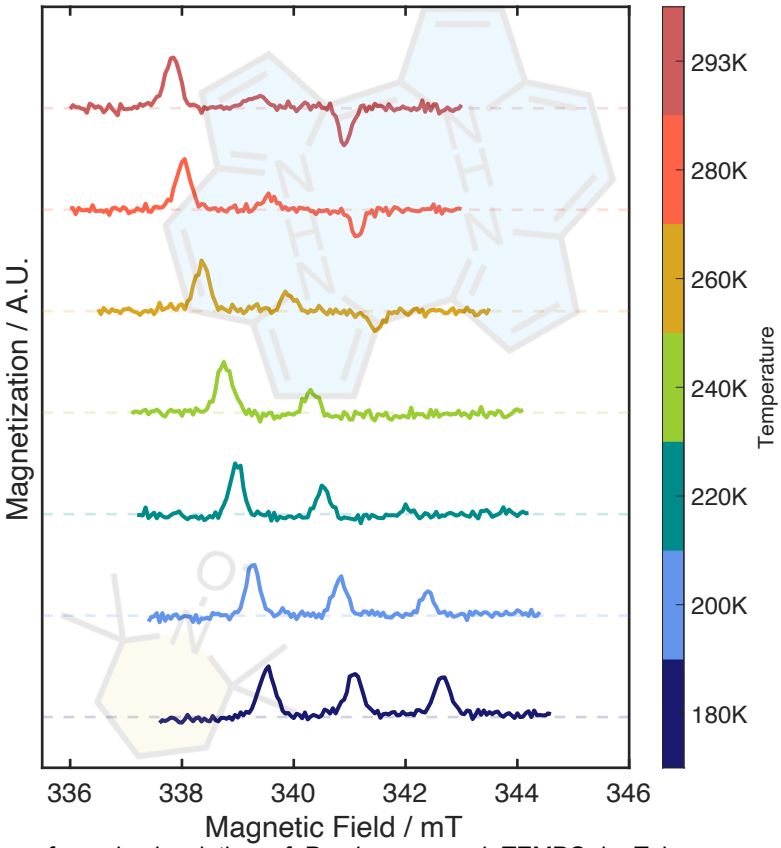
Chemically induced dynamic electron polarization (CIDEP) is a non-thermal distribution of spin-states which was previously observed in radical-triplet systems in liquid phase.[1-3] Different photophysical processes were proposed for generation of CIDEP such as the radical pair mechanism (RPM), triplet mechanism (TM), the radical-triplet pair mechanism (RTPM) as well as enhanced intersystem crossing (EISC) and electron spin polarization transfer (ESPT).
In this work, transient EPR (trEPR) was used for the detection of CIDEP on a TEMPO radical in a temperature range of 180-293 K, generated via direct interaction with photoexcited porphycene[4] freely diffusing in solution. Variable temperature measurements revealed significant hyperfine dependence on the polarization of TEMPO when polarized by porphycene. In comparable porphyrin systems, such as free-base tetraphenylporphyrin (H_2TPP) or its metallated analogue Zinc-tetraphenylporphyrin (ZnTPP), no such strong hyperfine dependence was observed.[5] The overall polarization on TEMPO is assumed to arise from EISC, ESPT as well as RTPM. This hyperpolarization could play an important role in possible applications for dynamic nuclear polarization (DNP), used in liquid state NMR.



of a mixed solution of Porphycene and TEMPO in Toluene. Porphycene was excited at 532 nm.

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Characterization of peroxy radicals in irradiated PTFE of industrial origin by means of EPR spectroscopy.

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Irradiated polytetrafluoroethylene (PTFE) is a material of significant industrial relevance due to its unique chemical and physical properties. Upon irradiation, used to break the polymer long carbon chains, perfluoroalkyl radicals are generated. In presence of oxygen these form peroxy radicals, which can undergo further reactions leading to carboxylic acids such as perfluorooctanoic acid (PFOA), a toxic compound regulated by the European Union. [1]

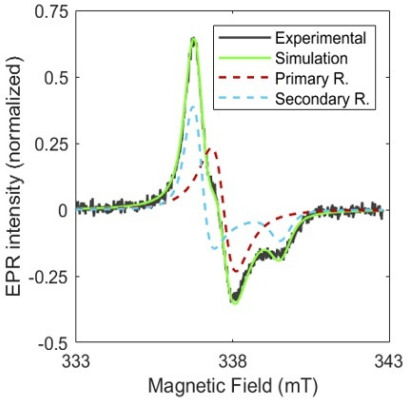

Figure 1. Room temperature cw-EPR spectrum of irradiated PTFE, with the simulation for the two radicals contributes

While electron paramagnetic resonance (EPR) spectroscopy has already been employed to study such radicals [1, 2], its application to industrial PTFE samples, particularly using pulsed EPR techniques, remains limited. In our study, we examined peroxy radicals in irradiated industrial PTFE using both continuous-wave and pulsed EPR methods. We investigated the nature of these radicals by analysing g-factors values and correlation times across different temperatures, and monitored radical concentration under various irradiation conditions, validating literature findings through simulations, as showed in Fig.1, and providing new insights into radical behaviour.

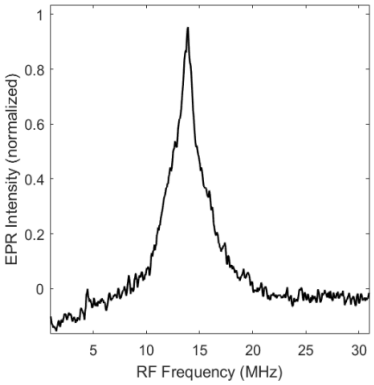

Figure 2. X—Band Davies ENDOR of irradiated PTFE, 10 K, 9.735 GHz

Using pulsed experiments, we probed for the first time in literature the interactions between paramagnetic centres and nearby nuclei. More specifically, two and three pulses ESEEM and Davies ENDOR experiments, showed in Figure 2, were employed for this goal. These techniques revealed information about the geometry and chemical environment in which the radicals form and persist, even over extended periods. We have observed signals consistent with interactions of nearby fluorine atoms with the radical.

To complement the experimental findings, quantum mechanical calculations have been performed and are ongoing, with the aim of understanding further the nature of the studied system and aiding the interpretation of the experimental results.

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