The 59th Annual International Meeting *of the* ESR Spectroscopy Group *of the* Royal Society of Chemistry

University Of Essex, Colchester
13th – 16th April 2026

RSC INTEREST GROUP
ESR SPECTROSCOPY

University of Essex

Contents

Welcome

It is our pleasure to welcome you to University of Essex for the 59th International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry. We have approximately 90 delegates registered for the conference with broad national and international representation, reflecting the thriving community centred upon electron spin resonance spectroscopy. It is particularly encouraging that we have a large contingent of student and postdoctoral scientists presenting oral contributions and posters, demonstrating the strength and future of our community. Our hope is that you enjoy the conference with its exciting programme of talks, posters and opportunities to network with colleagues.

The RSC ESR group are delighted to celebrate the 41st Bruker Prize awarded to Christiane Timmel for her outstanding and influential work studying the effect of magnetic fields on photoinduced electron transfer reactions, in particular the radical pair mechanism proposed to underlie avian magnetoreception. A very well-deserved prize for our previous Chair. Our Bruker Thesis prize is awarded this year to Annemarie Kehl for her work on developing simulation tools for the analysis of high-field 19F ENDOR. 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.

We extend our gratitude to JEOL for their steadfast support and sponsorship of the prize for best talk from an early career researcher, the competition for shortlisting grows in strength every year. Thanks also to our sponsors who will be pleased to meet with you at their exhibitions during the coffee breaks and evening receptions.

Special thanks go to the RSC ESR Spectroscopy Group who have provided support throughout the planning stages of this conference, and to Alison Claydon within the University of Essex Conference Team for her excellent management and advice.

We welcome you to Colchester, and wish you all enjoy the conference!

RSC-ESR Committee
April 2026
Colchester, UK

Conference Programme, Abstracts and Index

SUNDAY 12th April

If you booked an on-campus accommodation and arrive on Sunday, please go to the Information Centre (in Square 3) – people there will direct you to the right place to check in.

MONDAY 13th April

12:00	Registration Opening	EBS
13:00 – 15:00	Lunch 1 Coffee & Posters 1	Packed lunch will be served at EBS foyer Posters will be in EBS 2.65 and EBS 2.66
Session 1 (15:20 – 17:30), chaired by Jeanine Grüne: Conference opening, JEOL talks		**EBS 2.2**
15:20 – 15:30	Dimitri Svistunenko	Opening Remarks
15:30 – 15:50	Michael Wasielewski	S1_1: Molecular Diradical Spin Qubits in a Crystalline Host as a Platform for Quantum Sensing
15:50 – 16:10	Lorenzo Catini	S1_2: JEOL talk: Exploring spin-dependent processes in organic solar cells by Electrically Detected Magnetic Resonance
16:10 – 16:30	Sarah Chapman	S1_3: JEOL talk: A Rapid EPR–LC MS Workflow for Unmasking Hidden Radical Pathways in Complex Photochemical Reactions
16:30 – 16:50	Orit Nir-Arad	S1_4: JEOL talk: EPR at NMR Magnetic Fields: Insights into P1-DNP in Diamonds
16:50 – 17:10	Daniel Selby	S1_5: JEOL talk: Optical Dynamic Nuclear Polarisation in Solution-state Magnetic Resonance
17:10 – 17:30	Julian Stropp	S1_6: JEOL talk: Enhanced sensitivity and reduced spectral overlap in ENDOR spectroscopy with frequency-swept RF and MW pulses
Evening		
18:00 – 21:00	Dinner 1, followed by JEOL reception	EBS foyer

TUESDAY 14th April

8:45 – 9:00	Morning coffee/tea/fruit	EBS foyer
Session 2 (9:00 – 10:40), chaired by Janet Lovett		**EBS 2.2**
9:00 – 9:40	Plenary 1: Brian Crane	S2_1: In cell Flavoprotein Photoreduction as a Probe of Molecular Structure and Cellular Environment
9:40 – 10:00	Sergius Boschmann	S2_2: Distinct Valence States in Minimal FeFe-Hydrogenases
10:00 – 10:20	Gabriela Ionita	S2_3: Studying neutrophil elastase activity using peptide chain-functionalized radicals by EPR spectroscopy
10:20 – 10:40	Katrin Ackermann	S2_4: Validating a predicted unusual fold in a major streptococcal virulence protein – towards deciphering host-pathogen interactions inducing rheumatic heart disease
10:40 – 11:10	Coffee & Posters 2	EBS foyer, EBS 2.65 and EBS 2.66
Session 3 (11:10 – 12:35), chaired by Adam Brookfield: Poster presentations and sponsors' talks		**EBS 2.2**
11:10 – 11:40	FLASH POSTERS	
11:40 – 12.00	Jingwen Xia	S3_1: **CIQTEK:** Next-Generation EPR: Combining High-Performance Q Band Instrumentation with Artificial Intelligence Enhanced Spectral Processing
12:00 – 12:20	Timothy Keller	S3_2: **Bruker:** Broadband and Selective Inversion of Electron Spins
12:20 – 12:35	Austin Gamble Jarvi	S3_3: **High Q Technologies:** Applications of EPR to Biopharma: Structure, Dynamics, and Equilibria of a Monomer-Dimer System by Pulsed Dipolar Spectroscopy
12:35 – 14:00	Lunch 2	Silberrad

Session 4 (14:00 – 15:30), chaired by Paul Jonsen		**EBS 2.2**
14:00 – 14:30	Invited 1: David Britt	S4_1: mm-Wave (263 GHz) high power pulse EPR spectrometer and applications to high spin transition metal centers
14:30 – 14:50	Gediminas Usevičius	S4_2: Spiraling down: Versatile ESR using superconducting microresonator
14:50 – 15:10	Ilia Kaminker	S4_3: Measuring Electron Spin Dynamics under Magic Angle Spinning at 7 T on Hundreds of Microsecond Timescale
15:10 – 15:30	Marvin Lenjer	S4_4: Mims Electron-Nuclear Double Resonance (ENDOR) with microwave chirp pulses
15:30 – 16:00	Coffee & Posters 3	EBS foyer, EBS 2.65 and EBS 2.66
Session 5 (16:00 – 17:10), chaired by Alex Shread: Bruker Thesis talk		**EBS 2.2**
16:00 – 16:10	Marina Bennati (online transmission)	Bruker Thesis Prize Laudation
16:10 – 17:10	Annemarie Kehl	S5_1: Development of Analysis- and Simulation-Routines for ENDOR Spectroscopy
Evening		
18:30 – 22:00	Dinner 2, followed by drink reception and social evening	Silberrad

WEDNESDAY 15th April

8:45 – 9:00	Morning coffee/tea/fruit	EBS foyer
Session 6 (9:00 – 10:40), chaired by Alice Bowen		**EBS 2.2**
9:00 – 9:40	Plenary 2: Marilena Di Valentin	S6_1: Generation and transfer of long-lived electron spin polarization in chromophore-nitroxide molecular rulers
9:40 – 10:00	Hannah Eckvahl	S6_2: Detection of the Chirality Induced Spin Selectivity Effect in Achiral Donor Acceptor Molecules
10:00 – 10:20	Christian Teutloff	S6_3: Optically Tunable Spin-Spin Interactions in Diarylethene-Linked Porphyrin Architectures
10:20 – 10:40	Sebastian Michler	S6_4: EPR Spectroscopic Analysis of Pore Environments in Covalent Organic Frameworks by Dynamic Spin Probe Exchange
10:40 – 11:10	Coffee & Posters 4	EBS foyer, EBS 2.65 and EBS 2.66
Session 7 (11:10 – 12:40), chaired by Enrico Salvadori		**EBS 2.2**
11:10 – 11:40	Invited 2: Sofie Cambré	S7_1: Integration of triplet electron spin qubits in carbon nanotubes
11:40 – 12:00	Soyoung Oh	S7_2: Quantum Sensing in N@C60 Molecular Spin Systems
12:00 – 12:20	Samara Medina Rivero	S7_3: Magnetic Resonance Toolkit for Diradical Molecular Qubits
12:20 – 12:40	Fabio Donati	S7_4: All-electrical Coherent Control of a Single 4f Electron Spin
12:40 – 14:00	Lunch 3	Silberrad
Free afternoon What can I do in Colchester and area? See some recommendations in the Conference book.		
Bruker Lecture ceremony (17:30 – 18:40)		**Ivor Crewe lecture hall**
17:30 – 17:40	Gunnar Jeschke	Bruker Prize Laudation
17:40 – 18:40	Christiane Timmel Bruker Prize Talk	Bruker Prize: Excerpts from Our Travel Diary: Finding Our Bearings with Spin, Light, and Magnetic Compasses
Evening		
19:00 – 23:00	Dinner 3 (BBQ) Followed by Bruker Reception	Outside / Inside the Silberrad

THURSDAY 16th April

8:45 – 9:00	Morning coffee/tea/fruit	EBS foyer
Session 8 (9:00 – 10:40), chaired by Emma Richards		**EBS 2.2**
9:00 – 9:40	Plenary 3: Eric McInnes	S8_1: Magnetic Resonance Studies of Paramagnetic Rotaxanes
9:40 – 10:00	Gunnar Jeschke	S8_2: Interrogating catalysts at work with continuous microwave irradiation
10:00 – 10:20	Lisa Ebo	S8_3: SET – driven radical formation in nitroaromatics
10:20 – 10:40	Anatolii Vereshchagin	S8_4: Following redox processes in organic batteries by *in situ* EPR
10:40 – 11:10	Coffee & Posters 5	EBS foyer, EBS 2.65 and EBS 2.66
Session 9 (11:10 – 13:00), chaired by Marilena di Valentin		**EBS 2.2**
11:10 – 11:40	Invited 3: Claudia Avalos	S9_1: Predicting J-mediated Enhanced Intersystem Crossing in Chromophore-Radical Systems
11:40 – 12:00	Jeannine Grüne	S9_2: Spin-Dependent Pathways in Singlet Fission: The Role of High-Spin States in Luminescence
12:00 – 12:20	Naitik Panjwani	S9_3: Excitation Energy and Structural Control of Spin-State Formation in Singlet Fission
12:20 – 12:40	Enrico Salvadori	S9_4: Magnetic Properties of Surface-Bound ns^1 Species
12:40 – 13:00	Daniel Reta	S9_5: Unlocking Nitroaromatic Radicals: Characterisation & Reactivity
13:00 – 14:30	Lunch 4	Silberrad
Session 10 (14:30 – 15:50), chaired by Bela Bode		**EBS 2.2**
14:30 – 15:10	Plenary 4: Hannah Shafaat	S10_1: Investigating structure-function relationships in spin-coupled metallo-protein clusters using pulsed EPR spectroscopy
15:10 – 15:30	Jonathon Clark	S10_2: Investigating Key Radical Intermediates in Rhenium Based Photocatalytic CO_2 Reduction
15:30 – 15:50	Nicole Höfer	S10_3: Underestimation of Gadolinium-Based Contrast Agent Retention and Gadolinium Transchelation by Magnetic Resonance Techniques
15:50 – 16:30	Coffee & Posters 6	EBS foyer, EBS 2.65 and EBS 2.66
Session 11 (16:30 – 17:25), chaired by Eric McInnes		**EBS 2.2**
16:30 – 17:00	Invited 4: Alberto Collauto	S11_1: Fast acquisition of CW-EPR spectra to improve the time resolution of film-electrochemical EPR experiments
17:00 – 17:20	Yannik Limbach	S11_2: Probing limits of PELDOR / DEER distance measurements
17:20 – 17:25	Closing Remarks	
18:00 – 21:30	Conference Banquet	Wivenhoe House

WEDNESDAY AFTERNOON is a free session in the programme, allowing our delegates an opportunity to explore the University surroundings. Several suggestions are provided below. Please see a complete listing of activities available on the conference website page: https://www.esr-group.org/conferences/2026-conference-colchester/free-afternoon-wednesday/

Colchester town

Please use local transport to access the town centre. Highlights include:

- Colchester Castle – Norman keep on a Roman temple foundation
- Roman Walls & Balkerne Gate – among the oldest in Britain
- Dutch Quarter – picturesque historic streets
- Firstsite Arts Centre – free art exhibition and gallery

Wivenhoe Village

A short distance from the University, with a distinctly English character.

- Riverside walks along the River Colne
- Quiet streets and historic cottages

Colchester Zoo

Full details can be found on their website:
https://www.colchesterzoologicalsociety.com/
Tickets £18.10 if booked in advance (£25.85 on the door entry)
Transport: Bus 75 from Colchester Bus Station

Bruker Prize Lecture 2026

Professor Christiane Timmel

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 Interest Group committee is pleased to announce that the Bruker Prize for 2026 is awarded to Professor Christiane Timmel (University of Oxford, UK):

for her outstanding and influential work studying the effect of magnetic fields on photoinduced electron transfer reactions, in particular the radical pair mechanism proposed to underlie avian magnetoreception. Prof. Timmel has pioneered combinations of optical and magnetic resonance spectroscopies to probe magnetosensitive reaction kinetics in biological systems and synthetic molecular models. She has also made significant contributions to understanding spin polarization and spin delocalization in supramolecular structures for molecular electronics. Her comprehensive approach, seamlessly integrating experimental techniques with theoretical insights, along with her commitment to fostering teamwork and interdisciplinary collaboration, has led to significant advancements in the fundamental understanding of spin dynamics in chemical and biological systems. In addition to her scientific excellence, she has advanced the fields of ESR and spin chemistry both nationally and internationally through impactful mentorship and inspiring leadership.

The 2026 Bruker lecture is the 41st Anniversary of this prestigious prize, and we are excited to celebrate this milestone and Christiane's achievement at our Colchester conference in Spring 2026. The list of winners of the previous 40 Bruker Prizes is available here. We are grateful to Bruker for their longstanding support of this prize.

Excerpts from Our Travel Diary: *Finding Our Bearings with Spin, Light, and Magnetic Compasses*

Christiane Timmel

Centre for Advanced Electron Spin Resonance (CÆSR), Department of Chemistry, University of Oxford, Mansfield Road, Oxford OX1 3TA.

In *The Story of Spin*, based on his seminal lecture series, Sin-Itiro Tomonaga calls spin "the mysterious beast" and describes it as one of the most "subtle and ingenious designs of Nature". For those of us working in magnetic resonance spectroscopy and in spin chemistry, physics, and biology, this characterization resonates deeply: spin is both our subject and our tool — posing profound daily experimental and theoretical challenges while offering unprecedented insights into molecular structure and dynamics.

In this lecture, I will attempt to do justice to both the beauty and the complexity of spin. The systems discussed are inspired by Nature's ingenious designs, which have allowed us to elucidate one of the most elusive rules of life, to guide the development of new materials, and to contribute to improved sensitivity in spectroscopic techniques. At the heart of the talk lies the ESR-driven investigation of spin delocalisation and spin polarisation in supramolecular structures, as well as the study of spin-correlated radical pairs in artificial and protein-based magnetic compasses.

At its core, this lecture carries a simple message: I am the storyteller of a scientific diary, written by many hands and inspired by many minds, including mentors, collaborators, the broader community in which we work, and most of all the members of my group. I can only hope that, in telling it, I do justice to those who shaped it.

Bruker Thesis Prize 2026

The ESR Group of the Royal Society of Chemistry and Bruker Corporation are pleased to announce the winner of the 12th Bruker ESR Thesis Prize is

Dr Annemarie Kehl

Dr Annemarie Kehl completed her doctoral thesis, titled *"Development of Analysis- and Simulation-Routines for ENDOR Spectroscopy"*, at the Max Planck Institute for Multidisciplinary Sciences, Göttingen, under the supervision of Prof. Marina Bennati. Our international judging panel were impressed with the importance contribution her PhD thesis contributes towards the quantitative understanding of 19F hyperfine spectroscopy noting:

Lecture courses will have to be changed as a result of this research. The new simulation package for use with high resolution (and high field) ENDOR was employed in the very challenging problem of determining distance distributions in a biological sample. Essentially any research in future into "high resolution, high field" ENDOR would have this thesis and the publications that flow from it as required reading.

We look forward to hearing about this work in the thesis prize lecture which will take place during the conference at an award evening.

We are grateful to Bruker for their continued support of this prize, now in its 12th year. The prize is awarded annually, and now has an entry deadline of 1st October each year. For further details of the prize and a list of past winners please see our thesis prize page, where details of the next entry round will also be posted. Please join our mail list if you would like to be notified when applications are opened for the next Bruker Thesis Prize.

Development of Analysis- and Simulation-Routines for ENDOR Spectroscopy

Annemarie Kehl

Department of Chemistry and Applied Biosciences, ETH Zürich, Switzerland.

Electron nuclear double resonance (ENDOR) spectroscopy is a method of choice to detect the interactions between electron and nuclear spins to obtain structural information on for example biomolecules. Usually, the structural information is derived by comparison of magnetic parameters from experimental spectra with simulated spectra. Thus, the derived information is limited to the representation of the experiment by the simulation.

Advances in experimental setup constantly increase the resolution of spectra, *e.g.*, by enabling measurements at higher magnetic fields, with higher pulse power or with shaped pulses. This increases the information content of the spectra and more sophisticated and detailed simulations are required, especially when the effect of pulse sequences can no longer be approximated by a line shape function. A suitable method to directly quantify these effects are simulations of the spin dynamics.

Here, the development of a spin dynamics simulation routine for ENDOR spectra is described. It covers simulations of powder patterns and single crystals, couplings to multiple nuclei and different nuclear isotopes. It is also possible to include the pseudo-secular hyperfine interaction and relaxation effects in the simulation. Additionally, effects of the nuclear chemical shielding and inter-nuclear dipole-dipole couplings are considered. The latter effects are usually detected by nuclear magnetic resonance (NMR) spectroscopy but can now also be identified in ENDOR spectra. [1-3]

Applications are presented for the analysis of 19F-ENDOR spectra, where simulations are used to extract the hyperfine interaction of a 19F nuclear spin with an electron spin as a direct measure for the dipolar inter-spin distance. To identify the conformational flexibility of the investigated molecule, it is crucial to distinguish effects of the experimental setup such as the power broadening from those of the spin system, which include the chemical shielding anisotropy at high magnetic fields (9.4 T/263 GHz) and the influence of nuclear dipolar couplings. It is demonstrated that this is possible using spin dynamics simulations, allowing an identification of distance distributions.

[1] A. Kehl, M. Hiller, F. Hecker, I. Tkach, S. Dechert, M. Bennati, A. Meyer, *JMR* **2021**, *333*, 107091.
[2] H. Wiechers, A. Kehl, M. Hiller, B. Eltzner, S. Huckemann, A. Meyer, I. Tkach, M. Bennati, Y. Pokern, *JMR* **2023**, *353*, 107491.
[3] A. Kehl, L. Sielaff, L. Remmel, M. L. Rämisch, M. Bennati, A. Meyer, *PCCP* **2025**, *27*, 1415-1425.

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

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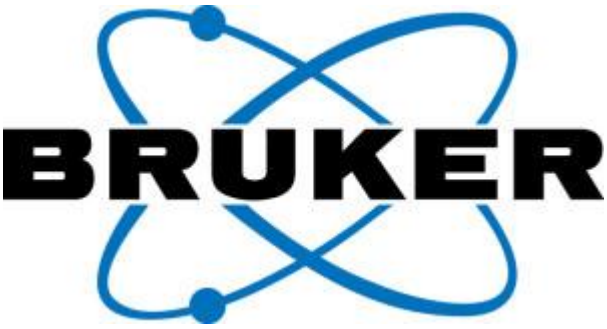
Conference Sponsors

The organisers and the RSC ESR Group Committee are indebted to all our sponsors for their generous support of our conference. Please visit our sponsors to hear what products they bring to ESR/EPR to assist you in exploring and developing your research interests: they are a valuable and contributing part of our community.

Gold Sponsors



Silver Sponsors

Silver Sponsors (continued)

Bronze Sponsors

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 open the conference and take place on Monday 13th April from 15:20 until 17:30.

This year's speakers are:

Lorenzo Catini (University of Oxford)
Exploring spin-dependent processes in organic solar cells by Electrically Detected Magnetic Resonance

Sarah Chapman (Imperial College)
A Rapid EPR–LC MS Workflow for Unmasking Hidden Radical Pathways in Complex Photochemical Reactions

Orit Nir-Arad (Tel-Aviv University)
EPR at NMR Magnetic Fields: Insights into P1-DNP in Diamonds

Daniel Selby (University of Manchester)
Optical Dynamic Nuclear Polarisation in Solution-state Magnetic Resonance

Julian Stropp (ETH Zürich)
Enhanced sensitivity and reduced spectral overlap in ENDOR spectroscopy with frequency-swept RF and MW pulses

Abstracts - talks

S1_1

Molecular Diradical Spin Qubits in a Crystalline Host as a Platform for Quantum Sensing

S. M. Kopp, J. R. Palmer, B. T. Phelan, K. R. Peinkofer, S. Nakamura, P. A. Watts, M. D. and M. R. Wasielewski

Department of Chemistry, Institute for Quantum Information Science Research and Engineering, and Center for Molecular Quantum Transduction, Northwestern University, Evanston, IL 60208-3113 United States.

Doping a luminescent tris(2,4,6-trichlorophenyl)methyl diradical ***m*(TTM)$_2$** into a host crystal of its diamagnetic precursor ***m*(HTTM)$_2$** creates a molecular color center with enhanced optical-spin interface properties important for quantum sensing. Optical polarization of the $|T_0\rangle$ sublevel of the diradical triplet ground state is achieved by spin-selective intersystem crossing from the $|T_+\rangle$ and $|T_-\rangle$ sublevels of the triplet excited state at ambient and cryogenic temperatures. Coherent spin control of ***m*(TTM)$_2$** doped into ***m*(HTTM)$_2$** using pulsed optically detected magnetic resonance (ODMR) spectroscopy results in a ten-fold improvement in ODMR contrast over that observed for randomly ordered ***m*(TTM)$_2$** using continuous-wave ODMR The diradical doped crystals achieve spin coherence times of 2.8, 3.4, and 7.4 μs at 294 K, 85 K, and 5 K, respectively. The diradical photoluminescence is sensitive to weak applied magnetic fields independent of temperature, excitation wavelength and dopant concentration, providing a promising pathway towards robust quantum sensing of anisotropic magnetic fields under ambient conditions.

Exploring spin-dependent processes in organic solar cells by Electrically Detected Magnetic Resonance

Lorenzo Catini, Luke Hanley, Jack Ovens, Claudia Tait

Department of Chemistry, University of Oxford, UK.

The efficiency of state-of-the-art organic solar cells is mainly limited by recombination of photoinduced charges generated on organic donor and acceptor molecules. The spin dependence of this process provides opportunities for new insights through Electrically Detected Magnetic Resonance (EDMR). In contrast to traditional EPR, magnetic resonance is detected through changes in current in fully operational devices caused by spin-dependent processes.[1] In addition to providing increased sensitivity, this detection method selectively probes spins directly involved in the current generation process.

In this work, we examined organic solar cells based on a range of organic donor:acceptor blends using a variety of pulse EDMR experiments at X- and Q-band frequencies. By addressing and coherently manipulating spins directly involved in charge recombination, we gain a comprehensive understanding of the nature, dynamics, and interactions of the states involved in this spin-dependent process.

The magnetic field dependence of the EDMR response, both following a single π pulse and through electrically detected spin echoes, allowed characterisation of the spectral signatures and relaxation properties of the spin states involved in spin-dependent processes. The presence of recombination of weakly coupled pairs of spins on donor and acceptor molecules was confirmed by the observation of spin-locking in Rabi nutation experiments and through double resonance methods selectively addressing the acceptor spin while monitoring the response of the coupled donor spin.[2] In addition to recombination of weakly-coupled spin pairs on donor and acceptor molecules, nutation experiments also revealed the presence of an alternative spin-dependent recombination mechanism involving the interaction of triplet states and single spins on donor and acceptor. This combination of pulse EDMR techniques provides important information on a key spin-dependent process, contributing to an improved understanding of the fundamental spin and photophysics of organic solar cells.

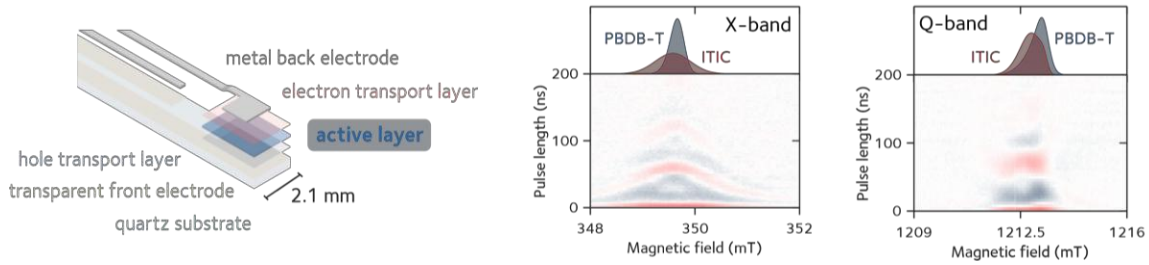


Figure 1. Schematic drawing of an organic solar cell fabricated for EDMR measurements; simulated spectral contributions of charged states on the donor PBDB-T and the acceptor ITIC as well as the results of Rabi nutation experiments performed at X- (left) and Q-band (right) on PBDB-T:ITIC solar cells.

[1] C. Boehme, *et al.*, *eMagRes*, **2017**, *6*, 83-100.

[2] A. J. Kupijai, *et al.*, *Phys. Rev. B*, **2015**, *92*, 245203.

A Rapid EPR–LC-MS Workflow for Unmasking Hidden Radical Pathways in Complex Photochemical Reactions

Sarah Chapman[1], Ben Robinson[2], Claire Donaldson[2], Laura Barter[1], Maxie Roessler*[1]

[1]*Dept. Chemistry, Molecular Sciences Research Hub, Imperial College London, UK.*
[2]*Syngenta, Jealott's Hill International Research Centre, Bracknell, Berkshire, UK.*

Photochemical reactions are notoriously difficult to decipher: they proceed *via* rapid, competing pathways, often generating short-lived radical intermediates that cannot be detected using conventional analytical methods.[1] This work delivers a facile, industry-accessible workflow that combines *in-situ* photoilluminated EPR with *ex-situ* LC-MS to characterise the mechanisms of photodegradation reactions. Building on the recent advances of Woodward *et al.* in *in-situ* EPR illumination,[2] the approach adapts these principles into a low-complexity setup compatible with standard EPR facilities and routine LC-MS workflows, enabling mechanistic insight without the need for bespoke instrumentation.

The methodology was developed using a model agrochemical, applying a simple, well-controlled system to mirror the early stages of the discovery pipeline.[3] The developed workflow begins with attempting direct EPR detection of intermediates, followed by indirect EPR detection of intermediates with DMPO spin trapping, and finally direct LC-MS detection of products, as shown in **Figure 1**. Within this framework, EPR analysis enabled selective identification of reactive oxygen species (ROS) for the characterisation of Type I and Type II photosensitisation pathways, and LC-MS analysis identified the stable reaction products. This combined approach revealed radical-ion mechanisms that are inaccessible to LC-MS alone, and linked the observed radical species to dominant product pathways such as dimerisation and rearrangement.

This work thereby establishes a practical, mechanistically powerful platform for characterising complex photoreactions. The integration of sensitive EPR detection with industry-prevalent LC-MS analysis provides an opportunity for early-stage mechanistic insight that is experimentally accessible and relevant for industrial research. The new mechanistic insights gained through this methodology could ultimately lead to better control of photochemical behaviour across a wide landscape of molecular systems, with agrochemicals showcased here as a representative example. The key contribution of this work is the creation of an experimentally simple EPR–LC-MS workflow that can deliver mechanistic photochemical insights in non-specialist environments.

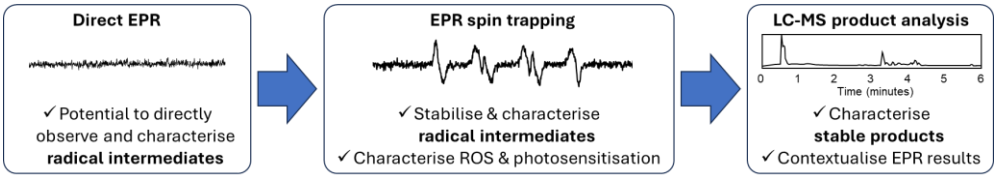


Figure 1. Methodology workflow for EPR and LC-MS characterisation of photodegradation mechanisms.

[1] A. Dashti, A. H. Navidpour, F. Amirkhani, J. L. Zhou and A. Altaee, *Chemosphere*, **2024**, *362*, 142792.

[2] A. W. Woodward, J. E. Bramham, A. Brookfield, A. P. Golovanov* and A. M. Bowen*, *Chemical Communications*, **2024**, *60*(8), 1012–1015.

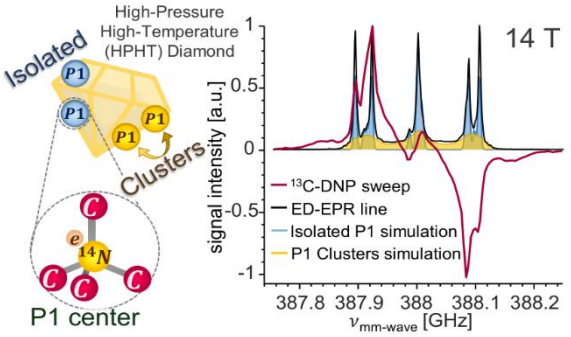
[3] M. D. David, *Pest Management Science*, **2017**, *73*, 692–699.

EPR at NMR Magnetic Fields: Insights into P1-DNP in Diamonds

Orit Nir-Arad, David H. Shlomi, Nurit Manukovsky, Alexander B. Fialkov, Ilia Kaminker.

School of Chemistry, Faculty of Exact Sciences, Tel-Aviv University, Israel.

High-field EPR (HF-EPR) has long been at the forefront of EPR method development owing to improved g-factor resolution, narrower lines in half-integer high-spin systems, and improved nuclear frequency separation in ENDOR. More recently, HF-EPR has been recognized as an indispensable tool for understanding Dynamic Nuclear Polarization (DNP) mechanisms.



EPR and ^{13}C-DNP spectra of P1 centers in diamond at 14 T in black and red, respectively. Overlayed with simulations of the isolated and P1 clusters.

DNP enhances NMR sensitivity by transferring polarization from electron spins to nuclear spins and is typically performed at high magnetic fields to benefit from increased NMR resolution. As a result, mechanistic insight into DNP is often limited by the absence of corresponding HF-EPR measurements. This limitation became particularly evident with the observation of unexpectedly efficient ^{13}C-DNP in diamond using substitutional nitrogen (P1) centers at magnetic fields up to 14 T, where solid-effect DNP is expected to be strongly suppressed [1–3]. Explaining this anomalously efficient P1-DNP required direct access to electron spin dynamics at these fields. This capability was enabled by the construction of a home-built 7 and 14 T dual DNP/EPR spectrometer operating between 8 and 300 K [4]. The instrument supports CW and pulsed EPR, electron-electron double resonance (ELDOR), and multinuclear DNP, enabling EPR and DNP measurements on the same sample under identical conditions.

HF-EPR measurements reveal that P1 centers electron spin distribution is more complex than inferred from low-field studies. In addition to isolated P1 centers, we identify a significant population of exchange- and dipolar-coupled P1 clusters, observed as a broad EPR component underlying the canonical P1 EPR spectrum [3]. Using pulsed EPR, ELDOR, and DNP, we show that this clustered population enables cross-effect-based mechanisms that underlie the efficient P1-DNP observed in HPHT diamonds [5].

These results demonstrate that HF-EPR measurements, made possible only by dedicated instrumentation, are indispensable for understanding and rationally optimizing DNP experiments at the magnetic fields used in modern NMR.

[1] D. Shimon, *et al.*, *J. Phys. Chem. C*, **2022**, *126*, 17777–17787.
[2] S. Bussandri, *et al.*, *J. Am. Chem. Soc.*, **2024**, *146*, 5088–5099.
[3] O. Nir-Arad, *et al.*, *J. Am. Chem. Soc.*, **2024**, *146*, 5100–5107.
[4] O. Nir-Arad, *et al.*, *J. Magn. Reson.*, **2024**, *360*, 107635.
[5] O. Nir-Arad, *et al.*, *J. Phys. Chem. Lett.*, **2025**, *16*, 10952–10960.

Optical Dynamic Nuclear Polarisation in Solution-state Magnetic Resonance

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A newly developed approach to solution-state dynamic nuclear polarisation (DNP) uses optical illumination instead of microwave pumping [1]. Upon illumination of a suitable dye, a triplet state is formed, which can undergo spin-selective quenching with radicals in solution to generate electron spin polarisation on the radical via the radical-triplet pair mechanism (RTPM) [2]. This chemically-induced dynamic electron polarisation (CIDEP) mechanism involves two steps: i) the triplet dye and radical diffuse together to form a doublet-quartet spin pair in an encounter complex, ii) this encounter-complex lives long enough to generate substantial polarisation of the radical's electronic transitions due to spin-allowed relaxation from the doublet manifold. Subsequent cross relaxation, that transfers the non-equilibrium electron polarisation to nearby protons, produces *in-situ* nuclear polarisation [1]. This approach polarises stable radicals, avoiding competitive kinetic decay processes that affect other CIDEP mechanisms.

The work presented applies a method of rapid mechanical shuttling of NMR samples on a benchtop spectrometer from low to high magnetic fields [3], to generate sensitivity enhancements in solution-state NMR using the RTPM. Continuous-wave illumination of the sample occurs using the benchtop's stray field, where the RTPM and cross-relaxation is most efficient, with sample transfer to the coil at higher magnetic field for improved chemical shift dispersion (see Fig. 1). Sample transfer is about 100 ms, minimising nuclear relaxation losses. We present preliminary findings showing optimal chemical systems and magnetic field strengths for generating polarisation. As well as time-resolved EPR data that gives insight into the salt and pH effects of the RTPM, first explored in DNP studies. Finally, we show this new DNP approach on dissolved substrates for the first time.

We gratefully acknowledge financial support for this work from the Royal Society [IEC\R3\213064] and Royal Society of Chemistry [E21-3124554325].

[1] M.W. Dale and C. J. Wedge, *Chem. Commun.* **2016**, *52*, 13221-13224.

[2] C. Blättler, F. Jent and H. Paul, *Chem. Phys. Lett.*, **1990**, *166*, 375-380.

[3] M. Reese, *et al.*, *Appl. Magn. Reson.* **2008**, *34*, 301–311.

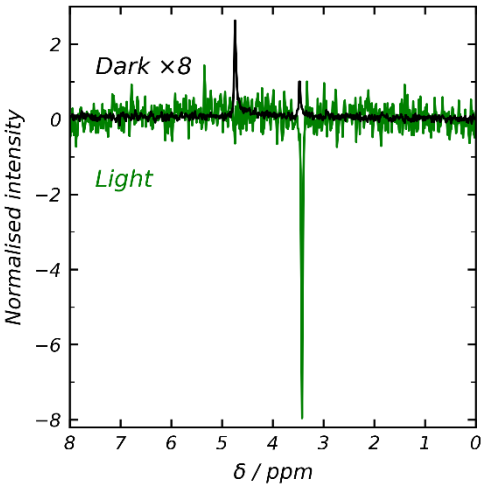

Figure 2: 1H NMR enhancement of glycine using the RTPM: illumination shows 8× DNP gain over 8 dark scans.

Enhanced sensitivity and reduced spectral overlap in ENDOR spectroscopy with frequency-swept RF and MW pulses

Julian Stropp[1], Hugo Karas[1], Nino Wili[2], Daniel Klose[1]

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Electron Nuclear Double Resonance (ENDOR) spectroscopy probes the geometric and electronic structure of paramagnetic centers, including transition metal complexes, using combined microwave (MW) and radiofrequency (RF) pulse sequences. However, its application to such systems is often limited by low sensitivity and severe spectral overlap arising from broad, anisotropic transitions of multiple nuclei.

To overcome these challenges, we upgraded an arbitrary waveform generator (AWG) based X-band EPR spectrometer to Q-band frequencies and included a dedicated AWG for the generation of shaped RF pulses to develop enhanced ENDOR experiments: First, broadband chirped RF pulses enhance sensitivity in frequency-domain ENDOR by exciting a larger fraction of nuclear spins, particularly for broad resonances of low-γ nuclei.[1] Second, chirped echo detection in Davies ENDOR (abbr. to CHEESY ENDOR) adds a hyperfine dimension to the spectrum without increasing acquisition time, thus separating overlapping features in 2D and simplifying spectral analysis.[2] Third, the implementation of chirped echo train acquisition provides additional sensitivity gains analogous to approaches in NMR.[3] Using ScoI-Cu(II), a metalloprotein essential in the biogenesis of mitochandrial complex IV in the respiratory chain, we demonstrate that the combination of all three approaches resolves spectral overlap from different types of nuclei (^{1}H, ^{15}N, ^{63}Cu). Moreover, CHEESY ENDOR separates hyperfine and nuclear quadrupolar interactions, allowing a more accurate determination of the spin Hamiltonian parameters and, consequently, the underlying electronic structure features. These results show that, despite the added complexity and ongoing research into chirp echoes, combining the developed methodologies substantially extends the applicability of ENDOR spectroscopy as demonstrated on systems with challenging target nuclei (^{27}Al, $^{47/49}$Ti, ^{63}Cu) that were previously inaccessible.[4]

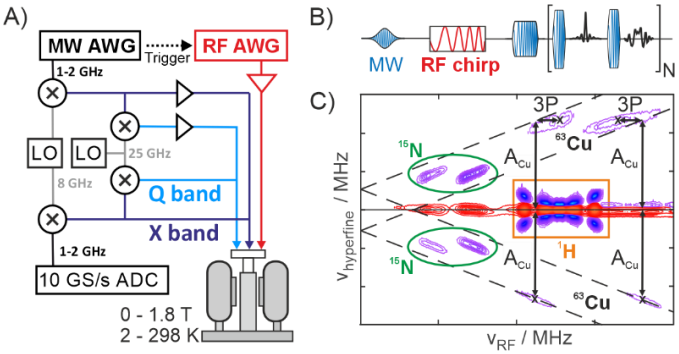

Figure 1. A) AWG-based EPR spectrometer with shaped MW & RF pulse excitation. B) CHEESY ENDOR sequence with chirped echo train acquisition. C) CHEESY ENDOR spectrum of the metalloprotein ScoI-Cu(II).

[1] Stropp, J., *et al*., *Magn. Reson.* **2025**, *6*, 33–42.

[2] Stropp, J., *et al*., *Phys. Chem. Chem. Phys.* **2025**, *27*, 25624-25635.

[3] Casabianca, L. B., *et al*., *JMR* **2014**, *242*, 197-202.

[4] Inoue, M., Stropp, J., *et al*. *J. Am. Chem. Soc.* **2025**, *147*, 19, 16438–1644.

In cell Flavoprotein Photoreduction as a Probe of Molecular Structure and Cellular Environment

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[2]*Weill Institute for Cell and Molecular Biology, Cornell University, Ithaca, NY.*

Electron-spin resonance spectroscopy of cellular samples has been limited by spin probe permeability and chemical stability. We have developed a new category of genetically encoded spin labels that are based on flavoproteins and applied them to several systems including: 1) the Aer transmembrane redox receptor in *E. coli* and 2) a small, modified flavodomain that can be fused to any protein of interest and expressed in bacterial and eukaryotic cells[1]. We extract information about the chemical form of the Aer flavin semiquinone radical *in vivo*, as well as the position and environment of the Aer flavin-binding domains by pulse-ESR techniques. The data provide insight into the biochemical mechanism of how Aer senses the activity of the electron-transport chain, whereas the structural data reveals higher order assemblies of Aer in the membrane important for cooperative signaling. Similarly, a small engineered Light Oxygen Voltage (LOV) domain functions as a genetically encoded spin probe when coupled to another protein. Upon photoexcitation, these probes form surprisingly stable radicals despite the reducing environment of the cell. We attach this photo-switchable domain to the histidine kinase CheA to establish that the substrate domains of CheA dimerize when bound to their receptor partners. Whole cell isotopic labeling (^{2}H or ^{15}N) and temperature variation were also carried out to improve the distance range measurement by 4P-DEER and to achieve the characterization of the spin systems by cw-ESR and hyperfine pulse ESR spectroscopy. Overall, this approach has the potential to reveal protein organization, localization, assembly and conformational processes directly in cells.

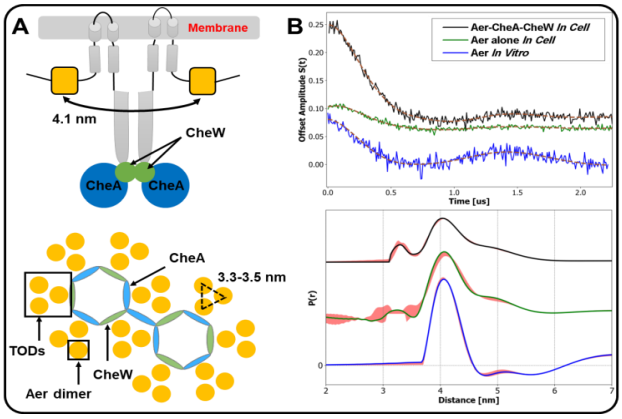

Figure 1. *In cell* ESR spin probes. (A) Schematic of the Aer receptor (sensing domains in yellow), higher-order assemblies below. (B) 4P-DEER time-domain data and distances reconstructions of Aer.B

[1] Chauviré T, Chandrasekaran S, Dunleavy R, Freed JH, Crane BR. Flavoproteins a native and genetically encoded spin probes for *in cell* ESR spectroscopy. *Nat Commun.* **2025**, *16*(1), 5406.

Distinct Valence States in Minimal FeFe-Hydrogenases

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[3]*Ruhr University Bochum, Bochum, Germany*

Redox-active enzymes often rely on metallocofactors to mediate complex oxidative and reductive transformations. Understanding the electronic structure of metallocofactors is key to manipulating these enzymes. By applying advanced EPR techniques, we can characterize paramagnetic states and track their evolution. Combined with biochemical and theoretical approaches, this enables new insights into the fundamental mechanisms of metalloenzymes.

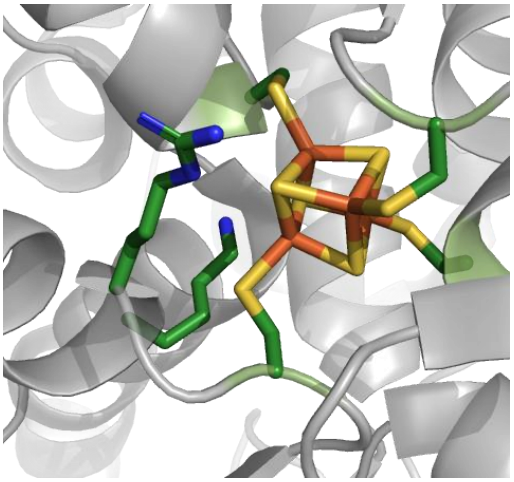

Figure 1. The singular apo [4Fe4S] cluster of *Cr*-HydA1, which can exhibit two distinct paramagnetic states when reduced.

To explore alternative mechanisms of electron transfer regulation, we investigated the minimal FeFe-hydrogenase *Cr*-HydA1, which lacks accessory FeS clusters.[1] There we could demonstrate the existence of distinct valence states arising from a single FeS-cluster. This concept is now being extended to a growing set of novel minimal hydrogenases. Based on this shared feature, we propose a new "redox switch" mechanism that operates in the absence of accessory FeS clusters. Our data suggest that structural heterogeneity and valence isomerism within the cubane cluster itself can serve as a regulatory element, tuning electron transfer and catalytic bias.

Our work on these distinct enzymes offers new insights into FeS cluster interactions and their role in enzymatic electron transfer, contributing to a broader understanding of FeFe-hydrogenases.

[1] Heghmanns, M.; Yadav, S.; Boschmann, S.; Selve, V. R.; Veliju, A.; Brocks, C.; Happe, T.; Pantazis, D. A.; Kasanmascheff, M. Distinct Valence States of the [4Fe-4S] Cluster Revealed in the Hydrogenase CrHydA1. *Angew. Chem. Int. Ed.* **2025**, e202424167. https://doi.org/10.1002/anie.202424167.

S2_3

Studying neutrophil elastase activity using peptide chain-functionalized radicals by EPR spectroscopy

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The enzyme/protease activity associated with various diseases and pathologies in different organs and tissues can be exploited in the field of Magnetic Resonance Imaging [1]. In this study, we investigated the enzymatic hydrolyse process in the presence of human neutrophile elastase (HNE) of the peptide MeO-Suc-(Ala)2-Pro-Val attached to TEMPO and two β-phosphorylated diastereoisomers radicals in the absence and in the presence of γ-cyclodextrin monitoring the changes in the EPR parameters. While no changes in spectral parameters were observed for the TEMPO derivative as a result of the enzymatic process, in the case of β-phosphorylated nitroxide radicals, the enzymatic process both in the absence and presence of cyclodextrin induces changes in the EPR parameters. The analysis of EPR spectra revealed that enzymatic hydrolysis led to a variation in the hyperfine splitting constant of 1.22 G in the system without cyclodextrin, while in the presence of cyclodextrin the variation in the splitting constant was 1.9 G for the radical shown in Figure 1. The spectra obtained for the system containing cyclodextrin show two components illustrating the simultaneous presence of the uncomplexed and complexed species. This leads us to conclude that the presence of cyclodextrin highlights the process of enzymatic hydrolysis. The EPR measurements were complemented by ESI-MS investigation to prove the reaction products of enzymatic process.

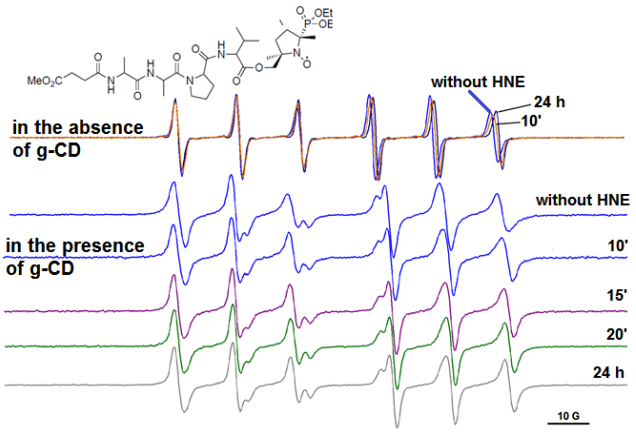

Figure 1. EPR spectra of the β-phosphorylated nitroxide in the absence of γ-CD and in the presence of γ-CD; effect of HNE.

[1] S. Seren, J.-P. Joly, P.Voisin, V. Bouchaud, G. Audran, S. R. A. Marque, P. Mellet, *J. Med. Chem*. **2022**, *65*, 9253−9266.

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.

Validating a predicted unusual fold in a major streptococcal virulence protein – towards deciphering host-pathogen interactions inducing rheumatic heart disease

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M proteins are major streptococcal virulence factors. These highly versatile proteins are involved in a broad range of human diseases ranging from relatively mild common infections ("strep throat") to serious, potentially life-threatening conditions including glomerulonephritis, necrotising fasciitis, or post-acute auto-immune sequelae such as rheumatic heart disease (RHD).

The extracellular M proteins are membrane-anchored and form long fibrillae consisting of parallel, homo-dimeric coiled coils.[1] Their hypervariable N-terminal region (HVR) is the basis for the *emm* typing, with about 275 types characterised to date and is also involved in binding a diverse range of host proteins, enabling for example immune evasion and adherence to host tissue. Despite their importance as virulence factors surprisingly little detail is known on M protein structure and the molecular basis for the plethora of interactions, and to date no full-length experimental high-resolution structure is available.

The rise of AlphaFold and thus, the availability of predicted atomistic protein structures, has made M proteins amenable for pulse dipolar EPR spectroscopy (PDS). Some *emm* types have been predicted to show a highly unusual, previously unseen protein fold reminiscent of the shape of a Hammerhead shark, making it an ideal target for characterisation and validation of topology by PDS. Interestingly, the presence of the fold seems to be associated with the ability to induce RHD through interaction of the HVR of the M protein with a particular region in collagen IV present in human cardiac base- ment membrane.[2]

Here, we use PDS to validate the predicted Hammerhead fold in streptococcal M3 protein and compare different predictions and a recently obtained crystal structure of a short cross-linked M3 construct with experimental PDS data.[3] We demonstrate that both, the fold and collagen binding capability are lost in a deletion construct lacking part of the HVR but still containing the PARF (peptide associated with rheumatic fever) motif.[4] We further show that sequence similarity to the HVR of M3 is not a prerequisite for the presence of the fold and outline the current working hypothesis for the host- pathogen interaction leading to RHD.

[1] Phillips GN; Flicker PF; Cohen C; Manjula BN; Fischetti VA. *Proc. Natl. Acad. Sci. USA* **1981**, *78*, 4689-4693.
[2] Tandon R; Sharma M; Chandrashekhar Y; Kotb M; Yacoub MH; Narula J. *Nature Reviews Cardiology* **2013**, *10*, 171-177.
[3] Ackermann K, Remmel L, Weiss H, Bode BE., *in preparation.*
[4] Dinkla K; Nitsche-Schmitz DP; Barroso V; Reissmann S; Johansson HM; Frick I-M; Rohde M; Chhatwal GS. *J. Biol. Chem.* **2007**, *282*, 18686-18693.

Next-Generation EPR: Combining High-Performance Q Band Instrumentation with Artificial Intelligence Enhanced Spectral Processing

Yang Zhou, Zhuoyang Qin, Yue Zhang, Zhiyu Jeff Sun, Zhifu Richard Shi, Kebiao Xu

This talk will be presented by Dr Jingwen Xia (Session 3)

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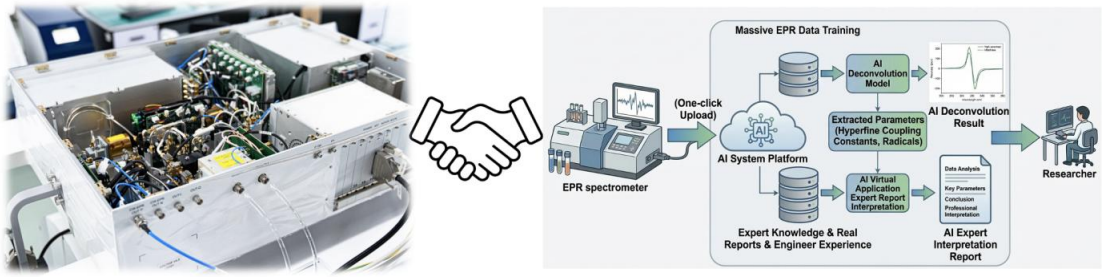

The advancement of Electron Paramagnetic Resonance (EPR) spectroscopy is increasingly defined by the convergence of robust hardware and intelligent software. While EPR remains a vital tool for probing paramagnetic centers, its broader adoption is often limited by instrument complexity and the steep learning curve of spectral analysis. Researchers at CIQTEK are addressing these barriers by developing high-performance hardware alongside the first dedicated AI model for EPR, collectively enhancing both the accessibility and the resolution of the technique.

On the hardware front, we have developed Q-band pulsed EPR system capable of 10 ns π/2 pulse wide-bandwidth excitation. Unlike traditional systems, this architecture utilizes a Solid-State Power Amplifier (SSPA), which offers superior longevity and significantly reduced maintenance compared to conventional vacuum-tube technology. This Q-band architecture effectively bridges materials chemistry and structural biology by offering a significant leap in data quality. By maximizing sensitivity and spectral resolution, it deciphers complex metal hyperfine couplings while leveraging orientational constraints to extract richer dipolar information for high-resolution DEER distance mapping.

Complementing these hardware-driven gains is a novel three-layer AI EPR model designed to streamline the entire investigative workflow from raw data to final publication. Trained on an extensive library of over 20,000 real and simulated datasets—achieving a test precision of 99.9% for simulations and 92% for complex, real-world samples—this digital assistant automates labor-intensive tasks such as spectral fitting, component characterization, and the generation of structured experimental reports. Beyond mere processing, the agent offers predictive guidance, suggesting specific follow-up experiments to ensure sample certainty and validate findings. By merging deep hardware integration with nuanced application expertise, this AI agent makes complex EPR data more approachable, empowering the community to significantly enhance scientific output in both quantity and efficiency.

By unifying high-bandwidth instrumentation with predictive analytics, we believe EPR can move beyond a niche specialized tool into a more impactful, high-throughput technology. This integrated approach not only increases the reliability of the data but also lowers the entry barrier for researchers in chemistry, biology, and materials science, ensuring the long-term vitality of magnetic resonance research.

Broadband and Selective Inversion of Electron Spins

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Recently, microwave pulse shaping has become a versatile tool for enhancing and expanding applications scope of EPR spectroscopy. From the perspective of structural biology application, pulsed EPR spectroscopy, particularly Double Electron Electron Resonance (DEER, aka PELDOR)[1] and Single Frequency Technique for Refocusing Dipolar Couplings (SIFTER)[2] techniques, have benefited from enhanced and uniformed excitation profiles of shaped pulses.[3-6] On the other hand, novel EPR applications, such as quantum information science and spin-based quantum technologies require not only broadband excitation, but also the ability to manipulate quantum systems (qubits) with high fidelity. Hence, probing the properties of qubits as well as preparation, control and read-out of specific qubit states have been of high interest for development of quantum devices and advancing quantum control techniques. EPR applications ranging from structural biology to spin-based quantum technologies that can be addressed by a single experimental platform needs a flexible, yet accurately controllable experimental architecture. To meet these demands, we developed microwave resonators with high uniformity and bandwidth of B1, where B1-bandwidth is controlled in accurate manner. For high fidelity operation, we integrated arbitrary waveform generator (AWG) using a concept of intermediate frequency (IF) that enabled efficient control of pulse excitation bandwidth, shape and resonance position across the EPR spectrum.

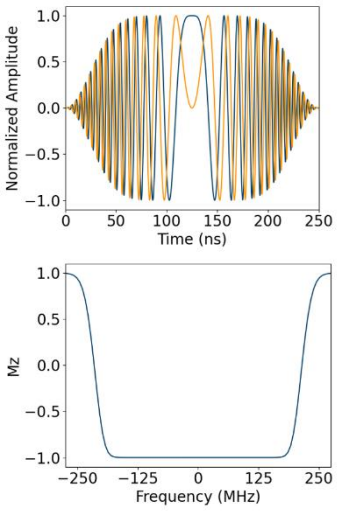

Figure 1. Broadband WURST pulse with a bandwidth of 500 MHz in time (top) and frequency (bottom) domains.

Applying WURST pulses that were adapted from NMR spectroscopy[7] (see Figure 1) and utilizing broadband Q-band loop-gap resonator and FT-EPR experiment architecture, we demonstrate broadband and selective inversion of electron spins coupled to nitrogen nuclei with a specific spin state using a diamond powder sample (see Figure 2). In addition, using broadband echo experiment architecture, we present efficient methods for probing properties of the electron spin system.

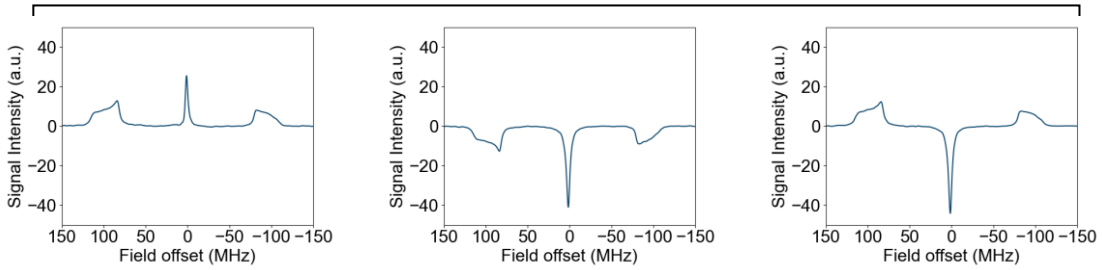

Figure 2. Fourier transformed broadband echo (left), broadband echo inversion (middle), and selective echo inversion (right) of P1 centers in diamond powder sample obtained at Q-band frequencies

Proposed strategies are applicable for wide range of quantum systems (qubits) and useful for advancement of novel quantum devices enabling efficient characterization of their properties and other quantum information science applications.

[1] Pannier, *et al.*, *JMR*. **2000**, *142*, 331.; [2] Jeschke, *et al.*, *Chem. Phys. Lett*., **2000**, *331*, 243.; [3] Doll, *et al.*, *Phys. Chem. Chem. Phys*. **2016**, *18*, 23111.; [4] Spindler, *et al.*, *Angew. Chem*. **2013**, *52*, 3425.; [5] Endeward, *et al.*, *J. Magn. Reson*. **2023**, *61*, 136-137.; [6] Schöps, *et al.*, *JMR*. **2015**, *250*, 55. ; [7] Kupče, *et al.*, *JMR. A* **1995**, *115*, 273.

S3_3

Applications of EPR to Biopharma: Structure, Dynamics, and Equilibria of a Monomer-Dimer System by Pulsed Dipolar Spectroscopy

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Pulsed Dipolar Spectroscopy (PDS), a branch of Electron Paramagnetic Resonance (EPR) spectroscopy that focuses on the measurement of interspin dipolar interactions, holds significant value for the investigation of protein-protein interactions (PPIs), capable of elucidating structural constraints, determining dynamic information, and counting coupled spins. Protein oligomerization is a specific type of PPI of great interest to pharmaceutical and drug-discovery industries. Because oligomerization influences and regulates many key protein categories such as enzymes, ion channels, and transcription factors, it plays a vital role in many biological and physiological processes that make appealing targets for therapeutic development. Therefore, understanding the mechanism of interaction is of significant interest to the scientific community.

Here, we apply Double Electron Electron Resonance (DEER), a robust and popular PDS technique, to investigate the dimerization of a homodimeric protein system. The distance distributions extracted from the DEER data are used to gain insight into the structure and dynamics of the dimeric complex, while careful analysis of the modulation depth of the dipolar traces reveals the populations of monomer and dimer states. Furthermore, we investigate the changes in these aspects as a function of buffer conditions and against the introduction of compounds that promote dimerization of the protein. These findings exemplify the capacity of EPR to contribute to questions across the PPI space, and the principles demonstrated here can be easily extrapolated toward other hot-topics within the biopharmaceutical industry, such as induced proximity and targeted protein degradation.

S4_1

mm-Wave (263 GHz) high power pulse EPR spectrometer and applications to high spin transition metal centers

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Department of Chemistry, University of California Davis

Pulse Electron Paramagnetic Resonance (EPR) spectroscopy provides powerful tools for examining species with unpaired electrons, such as organic radicals and metal ions, in a wide variety of interesting systems. However, the lack of high-power pulse amplifiers above approximately 100 GHz has limited its applicability at very high frequencies and magnetic fields. Here we describe the use of a new high frequency traveling wave (TWT) vacuum tube amplifier employed in a pulse EPR spectrometer operating over a wide frequency bandwidth centered at 263 GHz. The TWT power allows for pulse EPR without any resonator, which gives big advantages for sample volume and sample geometry. This novel instrument provides significant improvements in sensitivity and resolution when compared to lower frequency instruments. Very high frequency pulse EPR is of particular utility for studying spin S>1/2 species, given that large broadening effects of "zero-field splitting" interactions often dominate EPR spectra obtained at low frequency. Improvements obtained at 263 GHz are illustrated for a series of high spin (S=5/2) Mn(II) complexes. Future directions for the use of the instrument will be described.

Spiraling down: Versatile ESR using superconducting microresonators

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[2]London Centre for Nanotechnology, University College, London WC1H 0AH, UK [3]Dept. of Electronic & Electrical Engineering, University College London, London WC1E 7JE, UK

Electron spin resonance (ESR) is widely used across structural biology, quantum information science, solid-state physics, and chemical research. However, conventional ESR instrumentation typically relies on µL-mL scale samples to achieve sufficient signal-to-noise ratios, limiting studies of volume-restricted systems. Improving spin sensitivity without sacrificing compatibility with standard laboratory setups remains a central challenge.

In this work, we present a planar superconducting microresonator fabricated from high-temperature superconductor yttrium barium copper oxide (YBCO) and designed for operation at X- (Fig. 1) and Q-band frequencies (9.5 and 34 GHz, respectively), which adopts a spiral geometry. At X-band frequencies, spiral microresonator supports a microwave mode volume of approximately 7 nL. To ensure its straightforward implementation, we introduce a practical coupling strategy in which the planar microresonator is integrated into a standard 3D ESR cavity. This approach preserves compatibility with typical ESR instrumentation while enabling high magnetic fields (above 1 T) and temperatures up to 80 K under standard experimental conditions. The performance of the superconducting spiral microresonator is validated through pulsed ESR measurements on representative samples, including DEER, ESEEM, and ENDOR experiments.

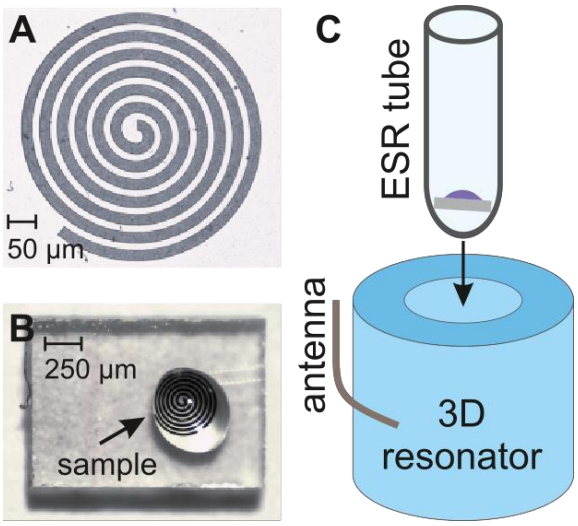
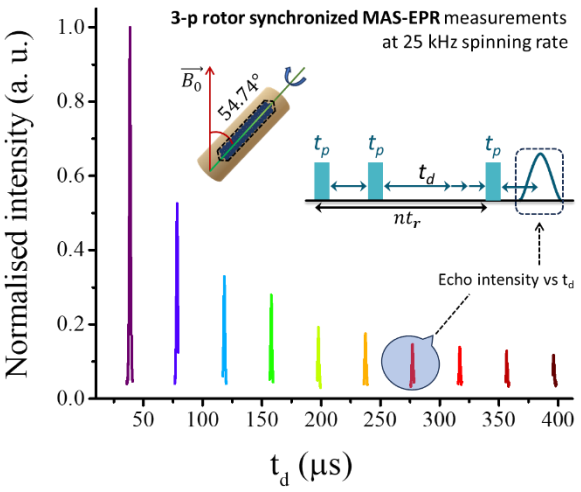


Figure 1: (a) Fabricated planar YBCO spiral microwave microresonator for X-band on a sapphire substrate. (b) Individual microresonator with an aqueous droplet containing nitroxide radicals. (c) The microresonator sits approximately horizontally at the bottom of an ESR tube, which is then loaded into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

Measuring Electron Spin Dynamics under Magic Angle Spinning at 7 T on Hundreds of Microsecond Timescale.

Ilia Kaminker

School of Chemistry, Faculty of Exact Sciences, Tel-Aviv University, Israel.



Recently, high-field EPR was demonstrated as an essential technique for the investigation of Dynamic Nuclear Polarization (DNP) – a prominent technique for signal enhancement in contemporary NMR. In the basis of DNP lies polarization transfer from an unpaired electron spin to neighbouring nuclear spins. Since DNP performance is condition-dependent, typical low-field static EPR experiments are of limited relevance for studying modern, high-field Magic Angle Spinning (MAS) DNP, necessitating high-field pulsed MAS-EPR instrumentation and methodology, currently undeveloped [1]. Recently, we reported the first high-field two-pulse MAS-EPR experiments at spinning rates up to 3 kHz [2], enabling observation of electron spin dynamics on a few-microsecond timescale. However, this timescale is shorter than a typical electron-nuclear polarization transfer in DNP.

Here, we demonstrate rotor-synchronized three-pulse stimulated-echo detected MAS-EPR experiments at spinning rates up to 37 kHz at 6.9 T, enabling observation of electron spin dynamics on the hundreds-of-microsecond timescale. This experiment provides insight into how MAS affects the stimulated echo decay rate, which is directly relevant to predicting MAS-DNP efficiency. Beyond DNP mechanism investigation, our results reveal the unique capability of MAS-EPR to separate EPR spectra of diamond P1 defects based on their anisotropy, achieved via the strong dependence of MAS-induced spin dephasing on the anisotropic line width. The experiments are accompanied by time-domain simulations that confirm the interpretation of the observed changes in the EPR line shapes.

[1] Hubrich, M.; Bauer, C.; Spiess, H. W. Magic-angle spinning electron paramagnetic resonance spectroscopy. *Chemical physics letters* **1997**, *273*, 259–264.

[2] Nir-Arad, O.; Fialkov, A. B.; Shlomi, D. H.; Manukovsky, N.; Mentink-Vigier, F.; Kaminker, I. High-field pulsed EPR spectroscopy under magic angle spinning. *Science Advances* **2024**, *10*, eadq6073.

Mims Electron-Nuclear Double Resonance (ENDOR) with microwave chirp pulses

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Electron-Nuclear DOuble Resonance spectroscopy (ENDOR) is an Electron Paramagnetic Resonance (EPR) method to measure hyperfine interaction between a paramagnetic centre and neighbouring nuclear spins, thereby providing structural information. In particular, ^{19}F Mims ENDOR has been established to measure inter-spin distances in the ångström to nanometer range.[1]

We present a modification of the Mims ENDOR experiment that uses microwave (MW) chirp pulses to enable broadband excitation in W-band (94 GHz) EPR spectroscopy and Fourier transform (FT) of the resulting stimulated echoes.[2] The method is demonstrated on a nitroxide-^{19}F model system and yields two-dimensional spectra that correlate hyperfine couplings with the EPR spectrum (Fig. 1). In contrast to standard, time consuming and costly orientation-selective ENDOR measurements, this approach requires just one experiment at a single EPR resonance field position. At the same time, the resolution in the EPR dimension is increased. This provides additional information on the orientation of the hyperfine coupling tensor and enables the direct observation of chemical shielding anisotropy at W-band frequency.

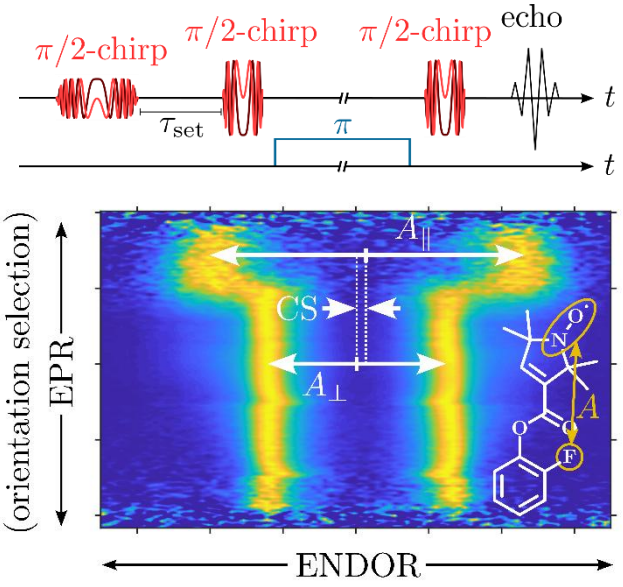

Figure 1. Pulse sequence of microwave chirp Mims (MCM-) ENDOR and W-band MCM ENDOR spectrum of the depicted ^{19}F-ENDOR model system.

While experiments at W-band or higher frequencies offer high EPR resolution, setups at lower frequencies are usually more readily available. We demonstrate two-dimensional FT ENDOR at Q-band frequency (34 GHz) using hard rectangular MW pulses. Therefore, the approach can also be used without high-field and pulse-shaping capabilities. Applying the method to more challenging samples and new sequences like Pulsed Dipolar Hyperfine Spectroscopy (PDHS)[3] is ongoing work.

[1] A. Meyer, *et al.*, *Angew. Chem. Int. Ed* **2020**, *59*, 373-379.
[2] M. Lenjer, *et al.*, *J. Magn. Reson.* **2026**, *382*, 108005.
[3] L. Sielaff, *et al.*, *Sci. Adv.* **2025**, *11*, eady5665.

Development of Analysis- and Simulation-Routines for ENDOR Spectroscopy

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Electron nuclear double resonance (ENDOR) spectroscopy is a method of choice to detect the interactions between electron and nuclear spins to obtain structural information on for example biomolecules. Usually, the structural information is derived by comparison of magnetic parameters from experimental spectra with simulated spectra. Thus, the derived information is limited to the representation of the experiment by the simulation.

Advances in experimental setup constantly increase the resolution of spectra, *e.g.*, by enabling measurements at higher magnetic fields, with higher pulse power or with shaped pulses. This increases the information content of the spectra and more sophisticated and detailed simulations are required, especially when the effect of pulse sequences can no longer be approximated by a line shape function. A suitable method to directly quantify these effects are simulations of the spin dynamics.

Here, the development of a spin dynamics simulation routine for ENDOR spectra is described. It covers simulations of powder patterns and single crystals, couplings to multiple nuclei and different nuclear isotopes. It is also possible to include the pseudo-secular hyperfine interaction and relaxation effects in the simulation. Additionally, effects of the nuclear chemical shielding and inter-nuclear dipole-dipole couplings are considered. The latter effects are usually detected by nuclear magnetic resonance (NMR) spectroscopy, but can now also be identified in ENDOR spectra. [1-3]

Applications are presented for the analysis of 19F-ENDOR spectra, where simulations are used to extract the hyperfine interaction of a 19F nuclear spin with an electron spin as a direct measure for the dipolar inter-spin distance. To identify the conformational flexibility of the investigated molecule, it is crucial to distinguish effects of the experimental setup such as the power broadening from those of the spin system, which include the chemical shielding anisotropy at high magnetic fields (9.4 T / 263 GHz) and the influence of nuclear dipolar couplings. It is demonstrated that this is possible using spin dynamics simulations, allowing an identification of distance distributions.

[1] A. Kehl, M. Hiller, F. Hecker, I. Tkach, S. Dechert, M. Bennati, A. Meyer, *JMR* **2021**, *333*, 107091.
[2] H. Wiechers, A. Kehl, M. Hiller, B. Eltzner, S. Huckemann, A. Meyer, I. Tkach, M. Bennati, Y. Pokern, *JMR* **2023**, *353*, 107491.
[3] A. Kehl, L. Sielaff, L. Remmel, M. L. Rämisch, M. Bennati, A. Meyer, *PCCP* **2025**, *27*, 1415-1425.

Generation and transfer of long-lived electron spin polarization in chromophore-nitroxide molecular rulers

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We report a new hyperpolarization mechanism in weakly-coupled triplet-radical spin systems where the chromophore and the nitroxide radical are held at fixed distances.[1] In this regime, the hyperpolarization of the stable paramagnetic centre can have a major impact in the enhancement of the sensitivity of EPR and NMR techniques, in primis light-induced Pulsed Dipolar Spectroscopy.[2]

Several model compounds based on a peptide-template have been considered, where the nitroxide position is progressively changed along the alpha helix (see Fig. 1), ranging from 1.4 nm to 4.2 nm. The chromophores employed are either a Zn-tetraphenylporphyrin, the corresponding metal free base, 2,6-diiodo-1,3,5,7-tetramethylbodipy or erythrosin B tethered at the extremity of the amino acid sequence. A helicene-based bridge has also been investigated.

In the presence of net polarization,[3] a spin-polarized radical signal is detected, whose intensity is shown to scale with the chromophore-radical distance as r^{-3}, in agreement with the behavior expected in the weak-coupling regime. Importantly, in the chromophore-nitroxide conjugates transfer of long-lived and long-distance electron spin polarization has been achieved, which is an important requisite for polarizing agents.

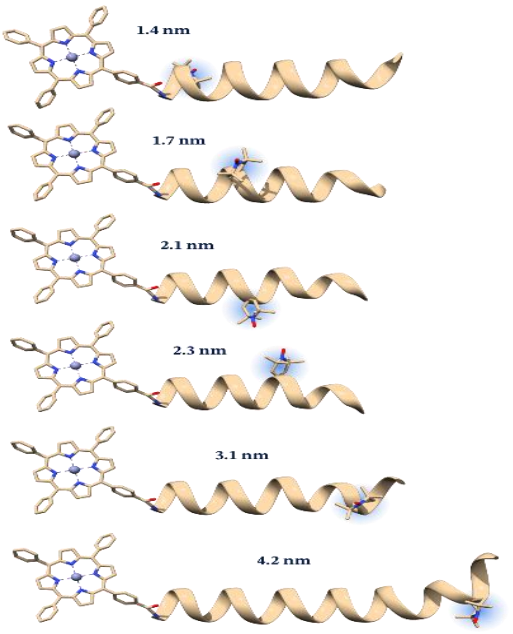

Figure 1. Molecular ruler: the increasing distance between the porphyrin chromophore and the hyperpolarized nitroxide moiety is depicted.

[1] M. G. Dal Farra, *et al.*, *Phys. Chem. Chem. Phys.* **2020**, *22*, 19982-19991.

[2] M. Di Valentin, *et al.*, *J. Am. Chem. Soc.* **2014**, *136*, 6582-6585.

[3] D. Panariti, *et al.*, *J. Chem. Phys.* **2025**, *162*, 114201-114212.

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

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[2]*Università di Parma, Dipartimento di Scienze Matematiche, Fisiche e Informatiche, I-43124 Parma, Italy*

The Chirality Induced Spin Selectivity (CISS) Effect can polarize electron spins as they travel through a chiral molecule[1]. Previous studies indicate that spin filtering can occur in systems consisting of achiral building blocks which undergo chiral supramolecular assembly.[2] Here, we expand on previous work detecting the CISS Effect in donor acceptor molecules using time resolved EPR (trEPR),[3],[4] by investigating the effect of induced chirality from the cholesteric phase of a liquid crystal[5] onto an otherwise achiral donor acceptor molecule.

The cholesteric phase of 5CB was prepared by addition of the chiral dopant R811 or its enantiomer S811. Compound 1 was then doped into these mixtures to form (1/5CB/R811) and (1/5CB/S811) (figure 1a). trEPR at 85 K was used to observe the radical pair resulting from photoexcitation of ANI in 1 aligned in 5CB/R811 and 5CB/S811, as well as in 5CB lacking the chiral dopant (1/5CB). The resulting spectra reveal distinct lineshape changes indicative of a strong CISS contribution (>80%) to the spin dynamics of radical pair formation in 1 when embedded in the cholesteric liquid crystals 5CB/R811 or 5CB/S811.

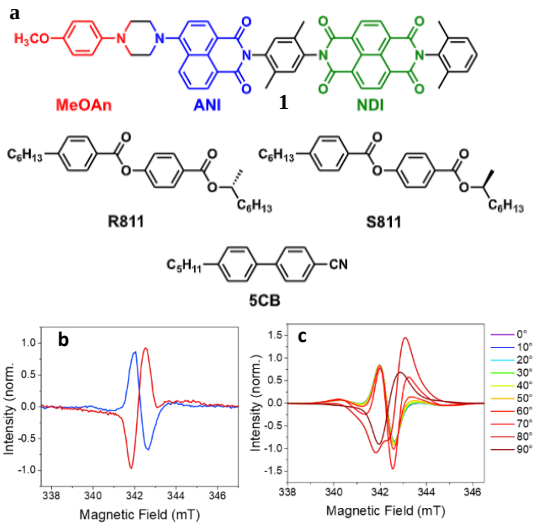

Figure 1 a) System under study, including the achiral donor acceptor molecule (1), the chiral dopants (R811 and S811) and the nematic liquid crystal (5CB) b) experimental trEPR spectra of 1/5CB (blue) 1/5CB/R811 (red) c) simulation of trEPR spectra of radical pair with increasing CISS contribution (χ = 0o, 0%, χ = 90o, 100%

These results demonstrate that CISS can be effectively induced by supramolecular chirality transfer in donor acceptor molecules that lack intrinsic molecular chirality. This expands the synthetic scope of donor acceptor molecules that can exhibit a CISS effect. It also opens the possibility of external environmental control over the spin polarization, which is essential for practical applications in quantum information science.

[1] B. P. Bloom, *et al*., *Chem. Rev.* **2024**, *124*, 1950-1991.
[2] A. K. Mondal, *et al*., *J. Am. Chem. Soc.* **2021**, *143*, 18, 7189–7195.
[3] H. J. Eckvahl, *et al*., *Science* **2023**, *382*, 197-201.
[4] H. J. Eckvahl, *et al*., *J. Am. Chem. Soc.* **2024**, *146*, 24125-24132.
[5] Y. Zhang, *et al*., *Chem. Eur. J.* **2023**, *29*(22), e202204039.

Optically Tunable Spin-Spin Interactions in Diarylethene-Linked Porphyrin Architectures

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The design of molecular platforms for quantum information science (QIS) demands multifunctional systems where spin states and interactions can be controlled on demand. In this work, we demonstrate the photomodulation of weak magnetic interactions in homometallic bis(metalloporphyrin) architectures bridged by a diarylethene (DAE) photochromic unit. The incorporation of copper(II) and oxovanadium(IV) porphyrins allows reversible switching between open and closed-ring isomers upon UV and visible light irradiation, enabling dynamic control over spin-spin distances and dipolar coupling.

Electron paramagnetic resonance (EPR) spectroscopy, including continuous-wave (CW) and pulsed techniques, was employed to investigate the spin properties of these systems in frozen solution. CW-EPR spectra reveal distinct changes in spectral linewidth upon photocyclization, indicating a shift in conformational flexibility and a reduction in metal-metal distance distribution. Double electron-electron resonance measurements further confirm the modulation of dipolar interactions, with distance distributions narrowing upon ring closure. Spin relaxation dynamics, assessed via inversion recovery and Hahn-echo experiments, show that coherence properties remain largely preserved despite photochromic switching, underscoring the robustness of these architectures for QIS applications.

These findings establish diarylethene-linked metalloporphyrin dimers as a versatile class of photoresponsive spin systems, where weak magnetic interactions can be optically tuned without compromising quantum coherence. The results pave the way for the development of molecular qubits and quantum gates with on-demand switchable coupling, advancing the integration of photochromic molecules into spin-based quantum technologies.

EPR Spectroscopic Analysis of Pore Environments in Covalent Organic Frameworks by Dynamic Spin Probe Exchange

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Martin Luther University Halle-Wittenberg, Faculty of Natural Sciences II, Institute of Chemistry, Von-Danckelmann-Platz 4, 06120, Halle (Saale), Germany.

The chemical fine-tuning of pore environments in covalent organic frameworks (COFs) is highly relevant for many of their applications. Continuous-wave electron paramagnetic resonance (CW EPR) spectroscopy was combined with spin probing to analyze the internal pore polarity and investigate pore-guest interactions in COFs. Two types of COFs with distinct topologies and pore characteristics – polar and non-polar – were synthesized and loaded with selected nitroxide spin probes from solution.

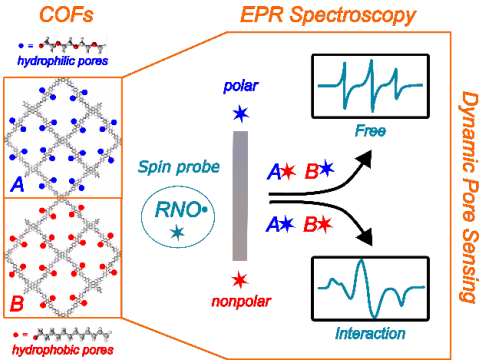

Figure 1. Experimental strategy of spin probing and analyzing COF pores with EPR spectroscopy.

The CW EPR spectra of the resulting mixtures were analyzed by spectral simulations, providing quantitative information on adsorption affinities and local concentrations of the guest radicals. The type and strength of pore-guest interactions were inferred from the rotational dynamics of the probes, while the hyperfine coupling constant allowed the quantification of the polarity difference between polar and non-polar pores. The results demonstrate the successful adsorption of various guest radicals into the pores with high local concentrations, leading to pore-induced Heisenberg exchange broadening and radical deactivation in certain systems. We observed a high thermodynamic affinity of non-polar spin probes toward both pore types, whereas polar probes showed a higher affinity to polar pores. Moreover, spectral signatures of multiple non-covalent interactions of the adsorbed radical species could be identified.

This study demonstrates the capability of CW EPR spectroscopy to characterize hydrated pore environments and pore-guest interactions with radicals, opening the door to a new analytical methodology for COFs and other porous materials.

Integration of triplet electron spin qubits in carbon nanotubes

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Theory and Spectroscopy of Molecules and Materials (TSM2), Physics Department, University of Antwerp, Belgium.

Optically addressable electron spin qubits are emerging as powerful platforms for quantum sensing, particularly when operable under ambient conditions.[1] While solid-state systems such as nitrogen-vacancy centers in diamond have demonstrated exceptional sensitivity through optical readout, their scalability and defect positioning remain challenging. Fully organic molecular qubits offer synthetic tunability and long coherence times, but often lack photochemical stability.[1]

Single-wall carbon nanotubes (SWCNTs), conceptually formed by rolling up a sheet of graphene in a cylinder, are very promising alternative platforms. Quantum confinement along the circumference leads to strongly bound excitons that show stable and narrow-band emission in the near-infrared. They are mechanically robust and show extreme photochemical stability under various conditions, which is rarely seen for organic molecular qubits. Interestingly, having all their atoms on their surface, they have demonstrated high sensitivity to their environment, already implemented towards biosensing.[2]

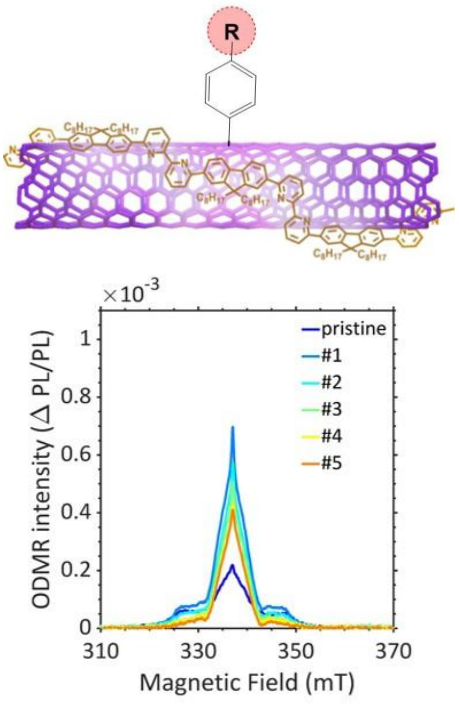

Figure 1. Schematic drawing of a functionalised (6,5) SWCNT; and corresponding triplet low temperature ODMR spectra.

In this work, we introduce optically addressable triplet spin qubits by engineered defects in SWCNTs. We demonstrate ODMR readout of these triplet states and how intersystem crossing can be tuned to enhance the ODMR contrast.[3-4] Finally, we will show recent results working towards ODMR at room temperature in the NIR and under ambient conditions, establishing SWCNT-based spin defects as a versatile and scalable platform for ambient-condition quantum sensing.

[1] C.A. Tesiman, *et al*., Surveying optically addressable spin qubits for quantum information and sensing technology, *arXiv*:2412.11232, **2026**.

[2] J. Ackermann, *et al*., Biosensing with fluorescent carbon nanotubes, *Angew. Chem. Int. Ed*. **2022**, *61*, e202112372.

[3] I. Sudakov, *et al*., Chirality dependence of triplet excitons in (6,5) and (7,5) single-wall carbon nanotubes revealed by optically detected magnetic resonance, *ACS nano* **2023**, *17*, 2190.

[4] J. Alejandro de Sousa, *et al*., Tuning intersystem crossing to triplet excitons in sp^3-functionalized (6,5) carbon nanotubes through defect density and functional groups, *ACS nano* **2025**, *19*, 36384.

Quantum Sensing in N@C60 Molecular Spin Systems Using Pulsed Electron Paramagnetic Resonance

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[2]*Faculty of Engineering and Science, University of Greenwich, Chatham Maritime, ME4 4TB, U.K.*
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[4]*The Korea Advanced Institute of Science and Technology (KAIST), Daejeon, 34141, Republic of Korea.*

Quantum technologies exploits quantum resources to outperform classical approaches. Among them, Quantum sensing leverages quantum properties, such as discrete energy levels, superposition, or entanglement to detect the minute physical quantities. A critical challenge, however, lies in maintaining high sensitivity to the target while preserving robustness against environmental noise, especially at room temperature.[1] In this context, molecular spins provide a promising platform for quantum sensing. Their design flexibility and integrability with electromagnetic source enable enhanced sensing interactions, leading to higher resolution and suppressed decoherence.[2]

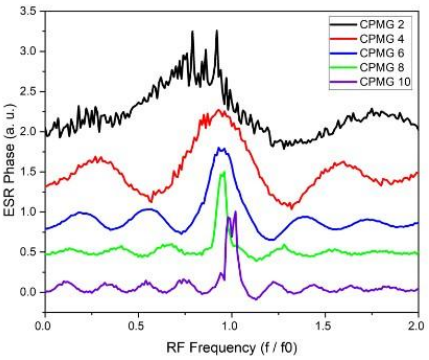

Figure 1. Magnetic field fluctuations are detected via phase accumulation of the electron spin echo in a CPMG multi-pulse sequence.

In this work, we demonstrate quantum sensing of magnetic fields using an ensemble of nitrogen-15-doped endohedral fullerene molecules (N@C60), dissolved in carbon disulfide (CS_2). The nitrogen atom I encapsulated within the fullerene cage exhibits an electron spin S=3/2, coupled to a nuclear spin I=1/2 of the 15N isotope. The encapsulating C60 structure offers a highly symmetric and inert environment, effectively decoupling spins from vibrational mode and leading long spin-lattice relaxation time. Notably, N@C60 exhibits exceptionally long phase decoherence times (up to 80 μs) at room temperature.[3] Using N@C60, we demonstrate quantum sensing of magnetic fields employing a multi-pulse electron spin echo sequence. By tuning the parameters of the pulse sequence, *e.g.*, pulse separation and number of pulses, we demonstrate the tuning of the sensing frequency and bandwidth. This work opens pathways for robust molecular spin-based quantum sensing platforms operating at ambient conditions.

[1] C. L. Degen, F. Reinhard and P. Cappellaro, *Rev. Mod. Phys*. **2017**, *89*, 035002.
[2] C.-J. Yu, S. von Kugelgen, D. W. Laorenza and D. E. Freedman, *ACS Cent. Sci*. **2021**, *7*, 712–723.
[3] J. J. L. Morton, A. M. Tyryshkin, A. Ardavan, K. Porfyrakis, S. A. Lyon and G. A. D. Briggs, *Phys. Rev. A* **2005**, *71*, 012332.

Magnetic Resonance Toolkit for Diradical Molecular Qubits

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[1]*TSM*[2]*, University of Antwerp, Belgium.*
[2]*National University of Singapore, Singapore.*
[3]*Donostia International Physics Centre (DIPC), Spain.*

Organic diradicals, *i.e.*, molecules with two unpaired electrons in their ground electronic state, have come back into spotlight in recent years due to their appealing properties for encoding electron spin qubits.[1] Since species bearing unpaired electrons are the natural domain of magnetic resonance techniques, the renewed interest in organic diradicals as Molecular Qubits (MQBs) has also boosted the use of these methods,[3-6] which are increasingly applied within the organic synthesis and materials chemistry community.

In this contribution, we show how magnetic resonance, in combination with optical spec- troscopy, can be employed to elucidate the feasibility of developing a spin-optical inter- face for an aza-triangulene diradical. On the one hand, Continuous Wave (CW-) Electron Paramagnetic Resonance (EPR) combined with (Time-Resolved, TR) Photolumines- cence are employed for revealing the suitability of the target diradical as a qubit system: optical addressability, high spin ground state and interactions between the electron spins. Pulsed-EPR, on the other hand, is not only employed to determine the spin-lattice relax- ation and the spin coherence times,[5] but also to disentangle how surrounding nuclear spins may affect these relaxation processes using HYSCORE experiments. Finally, Optically Detected Magnetic Resonance (ODMR) uniquely combines the spin manipulation under microwave irradiation of EPR with the high sensitivity of optical detection (*e.g.*, photoluminescence) enabling the traceability of the spin state during operation.[3, 4, 5, 6]

[1] A. Zhou, Z. Sun, L. Sun, *The Innovation*. **2024**, *5*, 100662.
[2] Y. R. Poh, D. Morozov, N. P. Kazmierczak, R. G. Hadt, G. Groenhof, J. Yuen-Zhou, *J. Am. Chem. Soc.* **2024**, *146*, 15549–15561.
[3] S. L. Bayliss, D. W. Laorenza, P. J. Mintun, D. E. Freedman, D. D. Awschalom, *Science* **2020**, *370*, 1309–1312.
[4] S. Gorgon, K. Lv, J. Grüne, B. H. Drummond, W. K. Myers, G. Londi, G. Ricci, D. Valverde, C. Tonnelé, P. Murto, A. S. Romanov, D. Casanova, V. Dyakonov, A. Sperlich, D. Beljonne, Y. Olivier, F. Li, R. H. Friend, E. W. Evans, *Nature* **2023**, *620*, 538– 544.
[5] S. M. Kopp, S. Nakamura, B. T. Phelan, Y. R. Poh, S. B. Tyndall, P. J. Brown, Y. Huang, J. Yuen-Zhou, M. D. Krzyaniak, M. R. Wasielewski, *J. Am. Chem. Soc.* **2024**, *146*, 27935–27945.
[6] R. Chowdhury, P. Murto, N. A. Panjwani, Y. Sun, P. Ghosh, Y. Boeije, C. D. Cordeiro, V. Derkach, S. J. Woo, O. Millington, D. G. Congrave, Y. Fu, T. B. E. Mustafa, M. Monteverde, J. Cerdá, G. Londi, J. Behrends, A. Rao, D. Beljonne, A. Chepelianskii, H. Bronstein, R. H. Friend, *Nat. Chem.* **2025**, *17*, 1410–1417.

All-electrical Coherent Control of a Single 4f Electron Spin

Yaowu Liu[1,2], Dasom Choi[1,2], Stefano Reale[1,2], Jeongmin Oh[1,2], Seorhin Choi[1,2], Fang Lei[1,2], We-hyo Seo[1,2], Arzhang Ardavan[3], Andreas J. Heinrich[1,2], Soo-hyon Phark[1,2], and Fabio Donati[1,2]

[1]*Center for Quantum Nanoscience, Institute for Basic Science, Seoul 03760, Korea.*
[2]*Department of Physics, Ewha Womans University, Seoul 03760, Korea.*
[3]*Department of Physics, University of Oxford, The Clarendon Laboratory, Parks Road, Oxford OX1 3PU, U.K.*

Electron spin resonance at the single-spin limit is emerging as a powerful route to study coherence, relaxation, and control in the most elementary magnetic objects [1]. Lanthanide atoms on ultrathin insulating films are particularly attractive in this context: the strong localization of their 4f electrons can yield long lifetimes [2] and weak coupling to environmental noise, while their adsorption geometry and ligand field allow chemical tuning at the atomic scale. Building on this surface-chemistry "knob set," we demonstrate an all-electrical route to coherently drive and read out a single 4f spin assembled on a surface.

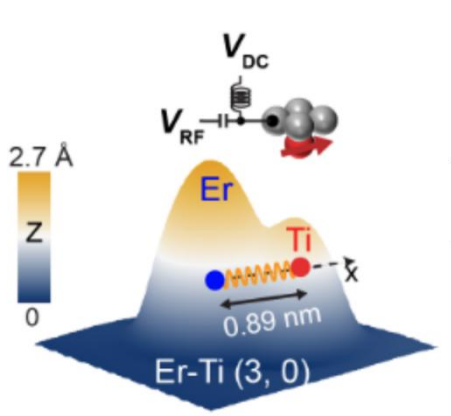

Figure 1: Electron spin resonance Scanning Tunneling Microscopy of a Er – Ti pair

Our platform is an Er–Ti atom pair constructed with atomic precision and measured by scanning tunnelling microscopy combined with electron spin resonance [3]. The Er ground state is engineered to couple efficiently to microwave fields [4], while the Ti–Er bond provides a controllable magnetic interaction channel. This approach enables sub-GHz Rabi frequencies, exceeding previously reported lanthanide-based surface qubits by roughly two orders of magnitude. By resolving the angular dependence of the spin transitions, we identify a control pathway that does not rely solely on conventional local driving fields. Instead, coherent driving is strongly enhanced by rotational modulation of an anisotropic spin–spin coupling tensor, activated by broken inversion symmetry in the adsorption complex and amplified by strong 4f spin–orbit interaction. This provides a concrete design principle: maximize driving efficiency by chemically and structurally engineering the interaction tensor (via adsorption symmetry, partner-atom selection, and controlled hybridization) rather than only increasing microwave field strength. Beyond a single-atom coherent ESR benchmark, this platform enables systematic studies of multiphoton transitions, designed couplings between individually addressable spins, and symmetry-engineered, interaction-driven control schemes that can break current gate-speed limits in solid-state spin qubits.

[1] Y. Wang, *et al*., Science **2023**, *382*, 87.
[2] F. Donati, *et al*., Science **2016**, *352*, 318.
[3] S. Reale, *et al*., Phys. Rev. B **2023**, *107*, 045427.
[4] S. Reale, *et al*., Nat. Commun. **2024**, *15*, 5289.

Excerpts from Our Travel Diary: Finding Our Bearings with Spin, Light, and Magnetic Compasses

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In *The Story of Spin*, based on his seminal lecture series, Sin-Itiro Tomonaga calls spin "the mysterious beast" and describes it as one of the most "subtle and ingenious designs of Nature". For those of us working in magnetic resonance spectroscopy and in spin chemistry, physics, and biology, this characterization resonates deeply: spin is both our subject and our tool — posing profound daily experimental and theoretical challenges while offering unprecedented insights into molecular structure and dynamics.

In this lecture, I will attempt to do justice to both the beauty and the complexity of spin. The systems discussed are inspired by Nature's ingenious designs, which have allowed us to elucidate one of the most elusive rules of life, to guide the development of new materials, and to contribute to improved sensitivity in spectroscopic techniques. At the heart of the talk lies the ESR-driven investigation of spin delocalisation and spin polarisation in supramolecular structures, as well as the study of spin-correlated radical pairs in artificial and protein-based magnetic compasses.

At its core, this lecture carries a simple message: I am the storyteller of a scientific diary, written by many hands and inspired by many minds, including mentors, collaborators, the broader community in which we work, and most of all the members of my group. I can only hope that, in telling it, I do justice to those who shaped it.

Magnetic Resonance Studies of Paramagnetic Rotaxanes

Eric J. L. McInnes

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Supramolecular chemistry has produced remarkable structures and functional molecules, as recognised by the award of the 2016 Nobel Prize for Chemistry to the pioneers of molecular machines. Most of this chemistry has been based on organic chemistry, for example, the rotaxanes based on long-chain molecules threading through macrocycles.

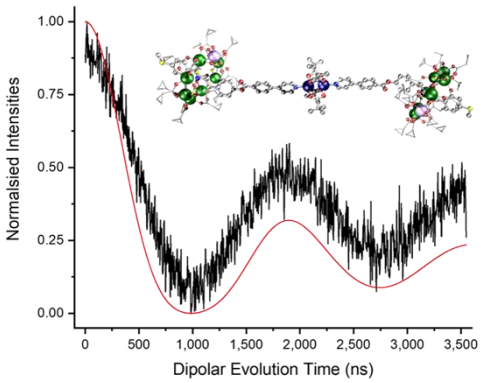

Figure 1. A [3]-rotaxane based on two paramagnetic metallocycles and an organic thread, DEER/PELDOR time trace.

We have been studying supramolecular structures where the molecular components are themselves complex inorganic molecules containing many paramagnetic transition metal ions.[1] Such molecules have attracted interest due to their unusual physics. In this talk I will describe systems based on molecules of general formula $(R_2NH_2)[M_7M'F_8(O_2CR')_{16}]$ (Figure 1). These complexes can be extended to supramolecular structures, for example using the M_7M' ring as the macrocyclic component of rotaxanes. Following such approaches huge structures containing hundreds of paramagnetic metal ions can be prepared. EPR and NMR techniques (and complementary methods) are used to explore the intra- and supra-molecular interactions which range from THz to MHz scales, and their solution chemistry.

[1] for a recent review see: S. J. Lockyer, G. F. S. Whitehead, G. A. Timco, E. J. L. McInnes, R. E. P. Winpenny, *Chem. Eur. J.* **2025**, *31*, e202501067.

Interrogating catalysts at work with continuous microwave irradiation

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Many catalytic reactions involve one-electron oxidation or reduction steps, meaning that spin state of the catalyst and reactant changes. If a paramagnetic spin state of either the catalyst or reactant is sufficiently stable, the reaction can be observed *in situ* by EPR spectroscopy or occasionally, ferromagnetic or antiferromagnetic resonance spectroscopy [1]. In particular, in the context of the Mars-Van Krevelen mechanism, where oxygen vacancies in a metal oxide support of the catalyst are involved, conductivity of the catalyst may change as well. Sample conductivity influences microwave reflection by the resonator, so that these changes are also observable with an EPR setup.

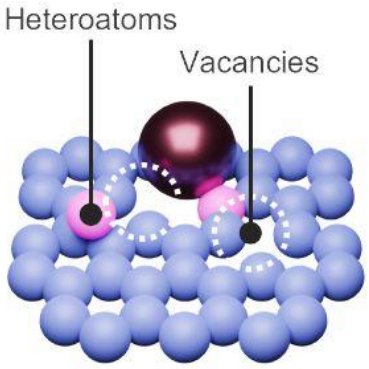

Figure 1. Even a single-atom (purple sphere) catalyst can be rather complex, as heteroatoms and vacancies in the support may be involved in the mechanism. Adapted from [1].

Interesting catalytic mechanisms are often complex and surprisingly often, catalysts feature more than one paramagnetic species. Revealing the active species requires observation at realistic reaction conditions, preferably in an *operando* mode, where product formation is observed as well. Here, we discuss application of our high-temperature operando EPR setup [2] to reactions where oxygen vacancies in the metal oxide support play a role [3] and showcase droplet EPR based on a microfluidic system for studying reaction kinetics in the liquid state [4]. We consider the question whether a conventional continuous-wave EPR spectrometer is the optimal instrument for such experiments.

[1] M. Agrachev, V. Giulimondi, I. Surin, S. Mitchell, G. Jeschke, J. Pérez-Ramírez, Electron paramagnetic resonance spectroscopy for the analysis of single-atom catalysts. *Chem Catalysis* **2024**, *4*, 101136.

[2] J. W. A. Fischer, F. Buttignol, A. Brenig, D. Klose, D. Ferri, V. Sushkevich, J. A. Van Bokhoven, G. Jeschke, Design principles of operando ultraviolet-visible and electron paramagnetic resonance spectroscopy setups for active site characterization in ion-exchanged zeolites. *Catalysis Today* **2024**, *429*, 114503.

[3] T. Pinheiro Araújo, G. Giannakakis, J. Morales-Vidal, M. Agrachev, Z. Ruiz-Bernal, P. Preikschas, T. Zou, F. Krumeich, P. O. Willi, W. J. Stark, R. N. Grass, G. Jeschke, S. Mitchell, N. López, J. Pérez-Ramírez, Low-nuclearity CuZn ensembles on ZnZrOx catalyze methanol synthesis from CO2. *Nat Commun* **2024**, *15*, 3101.

[4] T. Moragues, M. Agrachev, S. Mitchell, G. Jeschke, J. Pérez-Ramírez, A. J. deMello, Droplet-Based EPR Spectroscopy for Real-Time Monitoring of Liquid-Phase Catalytic Reactions. *Small Methods* **2025**, *9*, 2401771.

SET – driven radical formation in nitroaromatics

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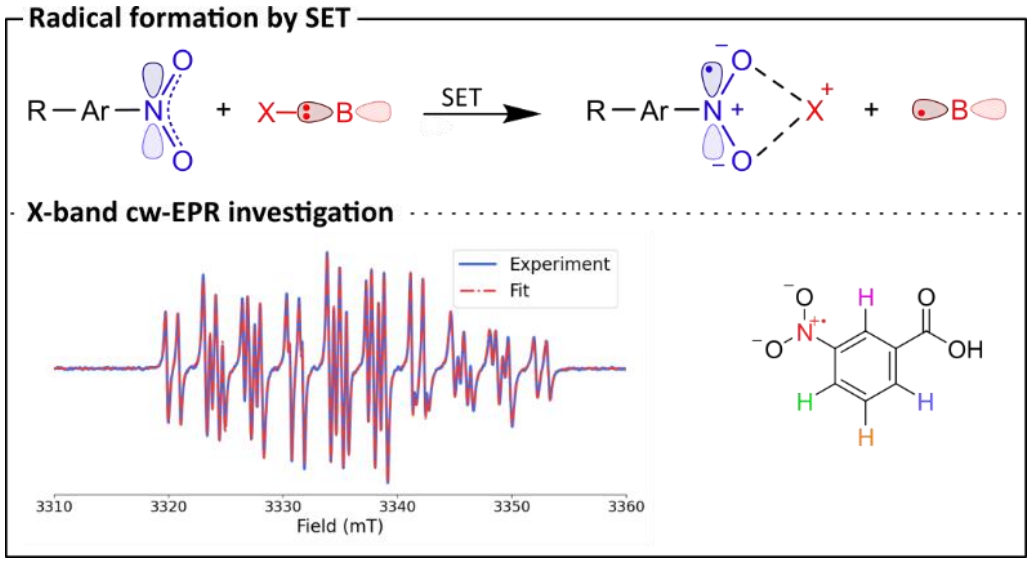
Knowledge of radical electronic structures enables the control of their properties and opens the potential of fine controlling their reactivity. Therefore, EPR is an unmatched technique, needed for the electronic structure characterization of organic radicals. However, the reactive nature of radicals and non-trivial preparational requirements limit the number of usable radical species until now. Enabling the generation of radical species under simple reaction conditions, employing available and inexpensive reactants, is therefore the key component for harnessing the extraordinary properties of organic radicals. In our recent work on nitrobenzene, we uncovered a radical formation process by a thermal single electron transfer (SET) from multiple anionic organo-bases1. I will show how the scope of this SET-driven radical formation can be expanded to the wider family of nitroaromatics, employing cw-EPR spectroscopy and DFT calculations. The understanding of the electronic structures of these radical pairs enables the utilization of radical compounds as reacting agents under mild synthetic conditions, laying the foundation for a new class of distinctive reaction mechanisms and thus unexplored opportunities in organic synthesis.



[1] Balahoju S., Bhattacharjee N., Lezama L., Lopez X., Salcedo-Abraira P., Rodríguez-Diéguez A., Reta D., Radical Formation by Direct Single Electron Transfer between Nitrobenzene and Anionic Organo Bases, *ACS Omega* **2025**, *10*, 23798-23807.

Following redox processes in organic batteries by *in situ* EPR

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Redox-conductive polymers are promising alternatives to inorganic-based energy storage materials due to their high energy density and fast redox kinetics.[1] However, their redox mechanisms, involving both polaron / bipolaron species and nitroxide radicals, make the analysis of charge transfer processes challenging. Electron paramagnetic resonance methods (*ex/in situ* cwEPR) offer direct insight into radical species, reaction mechanisms, and the local environment of redox centers.[2] Conducting *in situ* EPR experiments is challenging due to significant dielectric loss at microwave frequencies when using polar solvents and the need to maintain clear electrochemical responses. Traditional "flat-cell" and 3-electrode cylindrical cell provide experimental flexibility and can be tailored for specific samples.

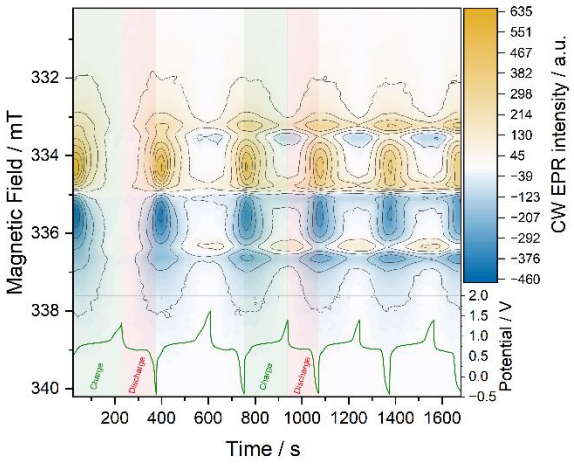

Figure 1. In situ cwEPR experiments coupled with a GCD overcharging process

This work focuses on operation properties of organic cathode materials based on TEMPO-containing Ni-Salen polymers. The cost-effective and accessible electrochemical cell design [3] for *in situ* EPR experiments in the X-band range (9-10 GHz) was used to test materials in organic electrolytes. The ability to obtain reliable, simultaneous electrochemical and cwEPR responses during the recharge process at various potential sweep rates was demonstrated. Full-spectrum cwEPR measurements enabled accurate assessment of the material's state of charge, while single-field-point measurements allowed precise determination of redox onset potentials. Cathodic material performance, its polymerisation and degradation processes were also analyzed, contributing to a deeper understanding of these transformations.

[1] A. A. Vereshchagin, *et al*., *Energies* **2022**, *15*(7), 2699.
[2] P. H. Rieger, *et al*., *J. Am. Chem. Soc.* **1963**, *85*, 683–693.
[3] A. A. Vereshchagin, *et al*., *J. Magn. Reson*. **2025**, 108010.

Predicting J-mediated Enhanced Intersystem Crossing in Chromophore-Radical Systems

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Chromophore-radical (C-R) systems have attracted attention in the spin physics community as potential candidates for dynamic nuclear polarization and quantum sensing due to their favorable optical and spin properties.[1] Similar to the NV^- center in diamond, the photoexcitation and subsequent relaxation of a C-R system may lead to a non-Boltzmann ground state spin polarization.[2] The magnitude of the triplet/radical exchange parameter J_{TR} has been predicted (via quasi-degenerate N-electron valence perturbation theory, QD-NEVPT2) to vary by orders of magnitude from fractions to hundreds of cm^{-1} in a series of similar pentacene based organic C-R systems, and is directly related to the degree of conjugation between the chromophore and radical electrons.[3] A wide range of J_{TR} values and different coupling regimes are possible, and the ability to reliably predict whether a given C-R system is likely to exhibit EISC based on ab initio excited-state coupling calculations would be highly beneficial for informed molecular design

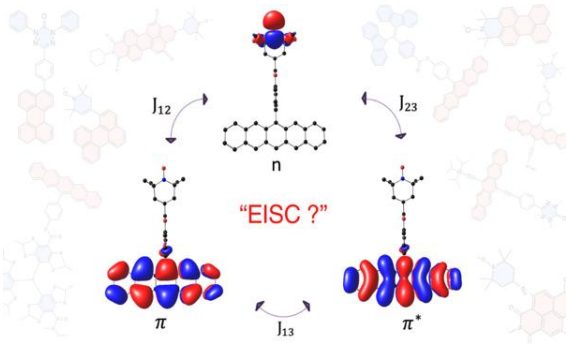

Figure 1. J-mediated enhanced intersystem crossing in pentacene-radicals.

In this work, we performed CASSCF/QD-NEVPT2 calculations to obtain the correct electronic wavefunctions and energies of electronic states in C-R systems. Using these results, we applied first-order perturbation theory to calculate a mixing term, κ, between the excited sing-doublet (SD_2) and trip-doublet (TD_1) states. Subsequently we compared these results to our own experimental datasets as well as those available in the literature which identify the presence or absence of J-mediated enhanced intersystem crossing. We then identify a threshold value of κ above which we expect to observe J-mediated EISC.

As part of this presentation, I will also discuss recent transient and pulsed EPR results on anthracene-sensitized pentacene-mono and bisnitroxide radical spin polarization. These experimental results are then discussed and compared to calculations in order to identify candidate structures that could lead to the observed intermolecular spin polarization transfer.

[1] Quintes, T.; Mayländer, M.; Richert, S.; *Nature Reviews Chemistry* **2023**, *7*, 75–90.

[2] Avalos, C. E.; Richert, S.; Socie, E.; Karthikeyan, G.; Casano, G.; Stevanato, G.; Kubicki, D. J.; Moser, J. E.; Timmel, C. R.; Lelli, M., *et al.*; *The Journal of Physical Chemistry A* **2020**, *124*, 6068–6075.

[3] Weiss, P. S.; Paz, A. S.; Avalos, C. E.; *Phys. Chem. Chem. Phys.* **2025**, *27*, 8052–8076.

Spin-Dependent Pathways in Singlet Fission: The Role of High-Spin States in Luminescence

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High-spin states are crucial in various organic applications, spanning from optoelectronics to quantum technologies and singlet fission (SF). This talk focuses on the formation and emission properties of spin states in SF systems. The principle is based on a photo-excited singlet exciton rapidly decaying into spin-correlated triplet pairs, before dissociating into free triplets. While extensive studies have addressed triplet formation and its role in photoluminescence, optical emission involving quintet states remains largely un- explored.

We focus on model systems of intra- and intermolecular singlet fission based on the SF-active chromophore diphenylhex- atriene (DPH). A particular focus will be on DPH-based oligomers, which allow tuneable geometry for accessing different spin regimes. We employ a set of unique spin-sensitive techniques to investigate high-spin state formation and emission, including electron paramagnetic reso- nance (EPR), optically detected magnetic resonance (ODMR), and optical spectros- copy, to probe the formation and evolu- tion of high-spin states [1].

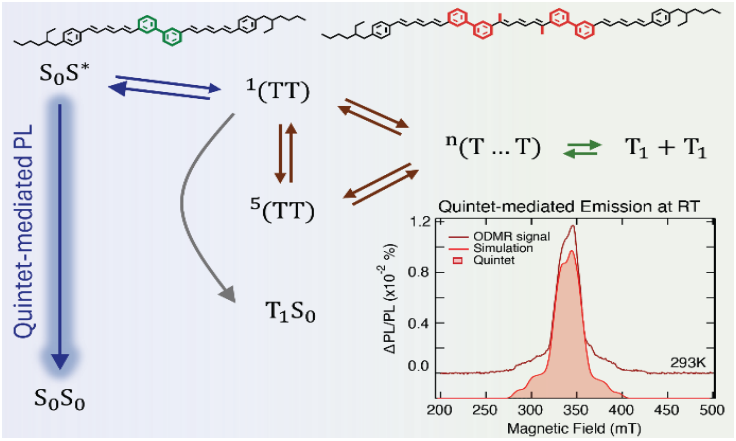

Figure 1. High-spin state dynamics in intramolecular singlet fission, including quintet-mediated emission up to room temperature.

We show that quintet states form robustly across all architectures and, remarkably, mediate photoluminescence that persists even at room temperature. However, the efficiency of triplet separation and involvement in luminescence is highly dependent on the molecular arrangement. These results establish a framework for controlling high-spin state evolution and emission in organic materials, with relevance for exciton multiplication and optically addressable spin states.

[1] Grüne, J., Montanaro, S., Bradbury, T. W., Sharma, A., Gillett, A. J., Gorgon, S., Myers, W. K., Behrends, J., Clark, J., Rao, A., Bronstein, H. & Greenham, N. High-Spin State Dynamics and Quintet-Mediated Emission in Intramolecular Singlet Fission. *Nat. Commun.* **2026**, *17*, 777.

Excitation Energy and Structural Control of Spin-State Formation in Singlet Fission

Naitik A. Panjwani[1], Kanad Majumder[2], Woojae Kim[3], Soham Mukherjee[4], Aisworika Mohanty[5], Sushil Lambud[6], Arka P. Ghosh[7], Jieun Lee[3], K.C. Krishnapriya[2], Kalishankar Bhattacharyya[7], Sandeep P. More[6], Jyotishman Dasgupta[5], Andrew J. Musser[4], Satish Patil[2], Robert Bittl[1]

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Singlet fission (SF) is the photophysical process in which photoexcitation of a molecule, through interaction with a neighbouring chromophore, leads to the formation of two free triplet (S = 1) excitons, proceeding via a correlated triplet–triplet (TT) pair state. This intermediate is initially formed in the singlet configuration, ^{1}(TT), and can evolve to populate triplet and quintet spin manifolds, ^{3}(TT) and ^{5}(TT) [1].

While SF has been extensively studied for its potential to enhance photovoltaic energy-conversion efficiencies, it is increasingly recognised as a versatile route to generating well-defined multi-exciton spin states. These include ^{3,5}(TT) manifolds and free triplet excitons, which provide a platform for studying spin-state evolution and multi-level spin control relevant to quantum sensing and dynamic nuclear polarisation [2]. Consequently, understanding how excitation energy and molecular structure govern the formation, population, and yields of these states is essential for directing SF towards applications.

Here we study a series of pentacene-based dimer systems using transient electron paramagnetic resonance (trEPR) spectroscopy to reveal how excitation energy and molecular structure govern SF-born quintet (^{5}TT) and triplet states. We show that excitation wavelength selectively alters quintet sublevel populations in a specific dimer [3]. By varying linker geometry, we show how planarity and orthogonality within the bridge control inter-chromophore coupling and its impact on quintet and triplet yields [4]. Finally, we examine the role of the ^{3}(TT)$\rightarrow T_1+S_0$ pathway, a loss mechanism in SF, where only a single free triplet exciton is formed. These results establish clear structure–property relationships for controlling SF-derived spin states, important across energy and quantum relevant technologies.

[1] L.R. Weiss, S.L. Bayliss, *et al.*, *Nature Phys.* **2017**, *13*, 176.
[2] Y. Kawashima, T. Hamachi, *et al.*, *Nat. Commun.* **2023**, *14*, 1056.
[3] W. Kim*, N. A. Panjwani*, *et al.*, *Cell Reports Physical Science* **2024**, *5*, 102045.
[4] K. Majumder*, S. Mukherjee*, N. A. Panjwani*, *et al.*, *J. Am. Chem. Soc.* **2023**, *145*, 38, 20883.

Magnetic Properties of Surface-Bound ns¹ Species

Enrico Salvadori[1], Yu-Kai Liao[1,2], Paolo Cleto Bruzzese[1], Bartolomeo Civalleri[1], Mario Chiesa[1]

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Paramagnetic species characterized by an ns¹ electronic configuration represent a fundamental class of atomic and molecular systems with a single unpaired valence electron. These species often act as key intermediates in reaction mechanisms because the high reactivity associated with the ns¹ configuration plays a crucial role in charge-transfer processes, surface interactions and ultimately in chemical bonding.

This electronic structure gives rise to well-defined magnetic, spectroscopic and reactive properties. In this contribution, we discuss the general physical and chemical behaviour of ns¹ paramagnetic species, with particular emphasis on transition metal and related open-shell systems.

From a general perspective, ns¹ species exhibit simple spin–orbital coupling schemes, and comparatively straightforward electronic spectra, making them ideal model systems for probing fundamental aspects of quantum magnetism and electron–nucleus interactions. Their magnetic response is dominated by the unpaired s electron, leading to minimal *g*-anisotropy and characteristic hyperfine interactions and long relaxation times.

Overall, the study of ns¹ paramagnetic species allows for general conclusions on the relationship between electronic configuration, magnetic behaviour, and chemical reactivity, highlighting their importance as benchmark systems for both experimental investigations and theoretical developments in atomic, molecular, and materials science.

[1] E. Salvadori, P.C. Bruzzese, E. Giamello, M. Chiesa, *Acc. Chem. Res.* **2022**, *55*, 24, 3706–3715.
[2] P.C. Bruzzese, Y.-K. Liao, L. Donà, B. Civalleri, E. Salvadori, M. Chiesa, *J. Phys. Chem. Lett*. **2024**, *15*, 28, 7161–7167.

Unlocking Nitroaromatic Radicals: Characterisation & Reactivity

Reta, D., Ebo, L., Zubillaga, I., Balahoju, S. A., Marvizon, J., Bhattacharjee, N., Lezama, L.

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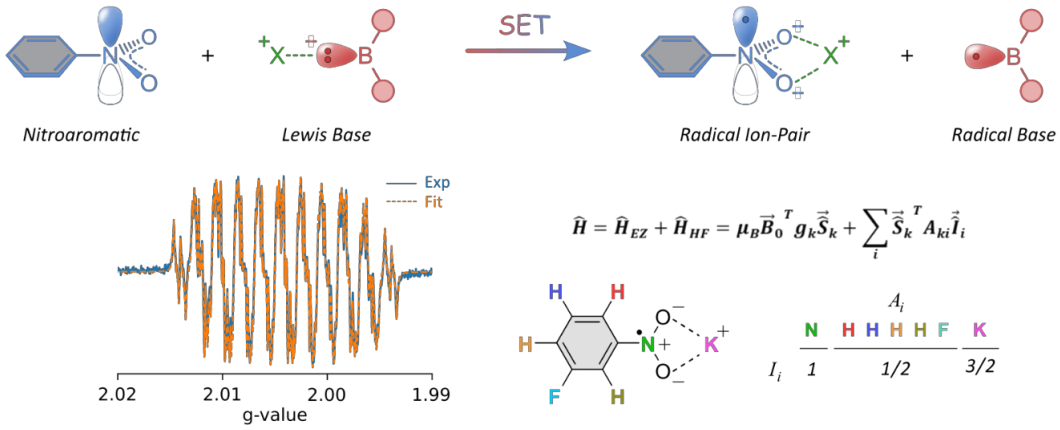
Organic radicals—metal-free molecules with unpaired electrons—exhibit unique magnetic and reactivity properties, enabling applications ranging from qubit implementations[1] to valuable chemical transformations.[2] However, their reactive nature and the synthetic challenges associated with their preparation impose strict structural and electronic constraints, limiting broader exploitation. Developing general strategies for radical formation under mild conditions, using readily available and inexpensive reagents, and applicable to a broad range of molecule, remains a key challenge.

Here, we present our efforts to establish nitroaromatic compounds as a versatile platform for radical formation, enabled by a single-electron transfer (SET) process from a wide range of anionic organo bases. Building on proof-of-concept studies of nitrobenzene,[3] and combining continuous wave X-band EPR spectroscopy, quantum chemical calculations, and synthetic approaches, we demonstrate that this SET-induced mechanism operates across a broad set of commonly used nitroaromatic compounds, including FDA-approved drugs – these findings suggest a previously overlooked prevalence of nitroaromatic radical species. We further show how this framework resolves contested reaction mechanisms[4] and enables the rational exploitation of SET-derived radical pairs to access valuable chemical transformations more efficiently.

Overall, our work highlights the untapped potential of SET-driven radical formation in nitroaromatic compounds and opens the door to extending radical properties to other Lewis acids.



Keywords: Organic Radicals, Single Electron Transfer, Lewis pairs, Nitroaromatics, Regioselectivity.

[1] Slota, M., Keerthi, A., Myers, W.K., *et al.*, Magnetic edge states and coherent manipulation of graphene nanoribbons. *Nature* **2018**, *557*, 691–695.

[2] Lu, Z., Ju, M., Wang, Y., *et al.*, Regioselective aliphatic C–H functionalization using frustrated radical pairs. *Nature* **2023**, *619*, 514–520.

[3] S. A. Balahoju, N. Bhattacharjee, L. Lezama, *et al.*, *ACS Omega* **2025**, *10*, 22, 23798–23807.

[4] Zhang, Z., Yue, S., Jin, B., *et al.*, *Para*-selective nitrobenzene amination lead by C(sp^2)-H/N-H oxidative cross-coupling through aminyl radical. *Nat Commun* **2024**, *15*, 4186.

Investigating structure-function relationships in spin-coupled metalloprotein clusters using pulsed EPR spectroscopy

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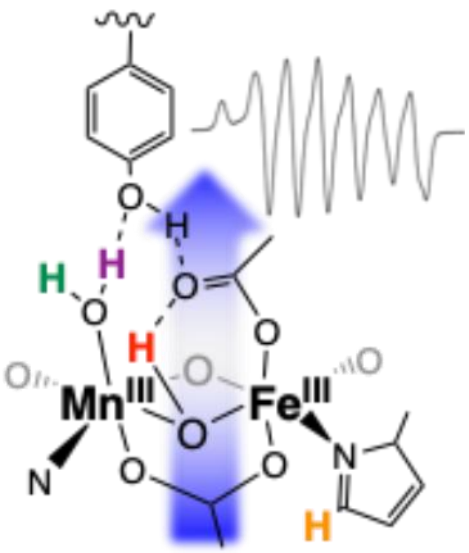

Figure 1. Active site of R2lox, the investigated in this work.

Nature employs multinuclear metalloclusters to carry out a range of multielectron chemical transformations, from oxygen activation and C-H bond oxidation to dinitrogen reduction and carbon dioxide fixation. Across these systems, finely tuned electronic interactions between the metals are essential to access the intended reactivity. However, it has been difficult to elucidate how reactivity is modulated by these interactions. In this work, we exploit a recently discovered class of heterobimetallic Mn/Fe oxidase proteins as a robust model platform to investigate how manipulating the metal-metal interactions impacts the oxidative reactivity. A series of point mutants have been generated to perturb the primary, secondary, and distal coordination environments around the cofactor. Continuous-wave and pulsed multifrequency electron paramagnetic resonance spectroscopy provides direct and indirect information on the electronic and geometric structure across the suite of R2lox mutants, with unnatural amino acid incorporation used to provide fine-grained information on hydrogen bonds. Further, we show that conventional approximations used for interpreting EPR spectroscopy on spin-coupled systems break down in the regime of intermediate-strength exchange interactions. This effect can be leveraged to yield high resolution information on hydrogen-bonding networks. Recent results suggest that the intermediate coupling regime found in native Mn/Fe enzymes contributes to the efficiency of coupling O_2 activation to C-H bond oxidation. These studies have implications for understanding the role of the protein environment in tuning intermetallic interactions and correlating those interactions with the resultant chemical potency of a spin-coupled cofactor, with relevance for understanding R2lox and related multimetallic systems.

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.

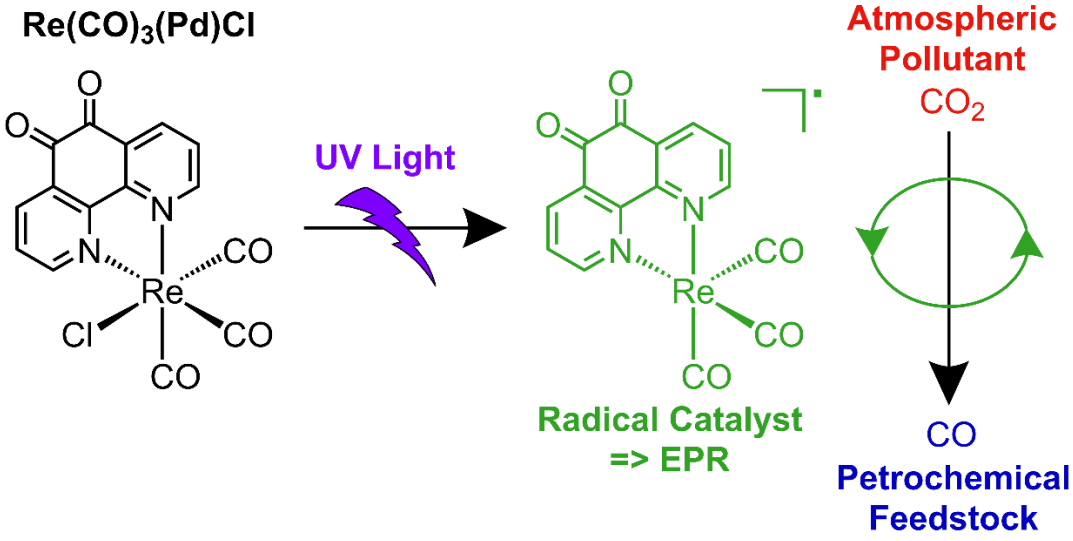

Figure 3: The proposed mechanism for generating the active catalyst in the reduction of CO2 to CO. Photolysis of Re(CO)3(Pd)Cl (left), by UV light, leads to formation of a radical based Re species which is proposed to be the active catalyst in the photoreduction of CO2.

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 and electronically characterised.

[1] L. J. Barrett, S. Rush and P. Vlahos, 'Chemistry of Carbon Dioxide Removal', *ACS*, **2024**.
[2] A. J. Morris, G. J. Meyer and E. Fujita, *Acc. Chem. Res*. **2009**, *42*, 1983-1994.
[3] H. Papp and M. Baerns, *Studies in Surface Science and Catalysis* **1991**, *64*, 403-461.

Underestimation of Gadolinium-Based Contrast Agent Retention and Gadolinium Transchelation by Magnetic Resonance Techniques

Nicole Höfer,[1] Lina Anderhalten,[2] Daria Dymnikova,[1] Julia Hahndorf,[3] Matthias Taupitz,[3] Heike Traub,[4] Christian Teutloff,[1] Carmen Infante-Duarte,[2] Robert Bittl[1]

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Gadolinium (Gd) retention after administration of Gd-based contrast agents (GBCAs) for magnetic resonance imaging (MRI) has been reported in various human tissues [1]. Linear GBCAs with lower kinetic inertness compared to macrocyclic GBCAs seem to lead to greater Gd accumulation, in particular under inflammatory conditions, which was shown by a prior study on experimental autoimmune encephalomyelitis (EAE), a common mouse model of multiple sclerosis [2].

Continuous wave electron paramagnetic resonance (cwEPR) and electron nuclear double resonance (ENDOR) spectroscopy at 94 GHz were used to investigate cerebellar biopsies of EAE and healthy control (HC) mice after *in vivo* administration of the linear GBCA gadopentetate-dimeglumine and the macrocyclic GBCA gadobutrol. The cwEPR lineshape as well as the ^{1}H ENDOR spectrum indicated a partial dissociation of the linear GBCA, and ^{31}P ENDOR detected phosphorus in the vicinity of retained Gd, suggesting an influence of phosphate-containing endogenous molecules in the release of Gd^{3+}. The macrocyclic GBCA was retained in its intact form [3].

However, a large discrepancy was found between the Gd concentration detected by EPR versus Gd concentrations measured by laser ablation inductively coupled mass spectrometry (LA-ICP-MS) in the case of linear GBCAs. A complementary MRI calibration experiment also severely underestimated the amount of retained Gd in tissue from specimen treated with linear GBCA, supporting the hypothesis of solid and relaxation-inactive inorganic Gd deposits which are invisible to EPR [3]. Again, this effect was most prominent in inflamed tissue. Preliminary experiments to redissolve and uncover these deposits were performed by adding strongly chelating complexes.

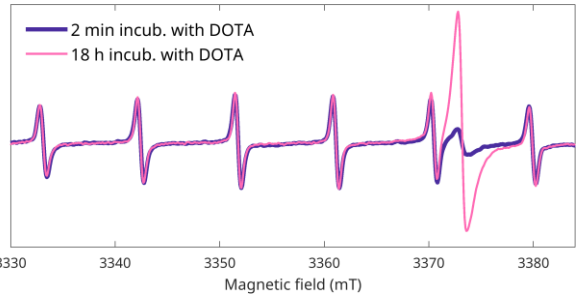

Figure 1. 94 GHz cwEPR on gadopentetate-treated EAE mouse brain incubated with DOTA.

This work was supported by DFG, CRC 1340 Matrix in Vision.

[1] M. Kobayashi, *et al*., *Radiology* **2021**, *300*(3), 559-569.
[2] L. Anderhalten, *et al*., *Invest. Radiol.* **2022**, *57*(10), 677-688.
[3] L. Anderhalten,* N. Höfer*, *et al*., *Invest. Radiol.* **2026** (*accepted*).

Fast acquisition of CW-EPR spectra to improve the time resolution of film-electrochemical EPR experiments

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Operando film-electrochemical EPR spectroscopy (FE-EPR) [1] provides unique mechanistic details of electrocatalytic reactions by enabling the real-time characterisation of paramagnetic intermediates.

Investigation of fast electron transfer processes, made possible by the direct control offered by film electrochemistry over the electron flow between the electrode and the surface-immobilised redox-active species, requires a time resolution for the EPR acquisition in the range of at least hundreds of milliseconds. In contrast to this, the acquisition time of a single CW-EPR spectrum is above 4 seconds even for narrow field scans [1, 2]. The resulting loss in time resolution caused by the change in the electrochemical response during the EPR measurement currently restricts the applicability of the technique.

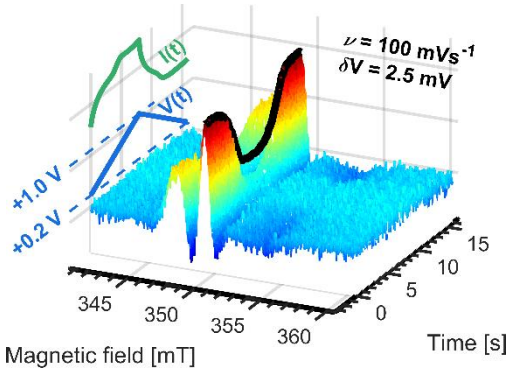

Figure 1. 2D dataset obtained using the proposed EPR acquisition method, demonstrating the ability to follow fast electrochemical processes.

In this work, we demonstrate that the CW-EPR acquisition time can be reduced to ~100 ms if the setup-scan coils that commercial EPR spectrometers are equipped with are used to generate the magnetic field sweep. The improved acquisition scheme enables the measurements of spectra of up to 20 mT-wide with virtually no delay between consecutive scans and relies on equipment already available in many laboratories.

An application of the proposed acquisition scheme is illustrated (Figure 1) for the characterisation of functionalised carbon nanotube electrodes for nitroxide-mediated alcohol oxidation [2].

[1] M. Seif-Eddine, S. J. Cobb, Y. Dang, K. Abdiaziz, M. A. Bajada, E. Reisner, M. M. Roessler, *Operando film-electrochemical EPR spectroscopy tracks radical intermediates in surface-immobilized catalysts*, *Nat. Chem.* **2024**, *16*, 1015–1023.

[2] Y. Dang, M. Seif-Eddine, Z. Ying, M. Shaffer, M. M. Roessler, *Carbon Nanotube Electrodes as a Versatile Platform for Operando Film-Electrochemical EPR Spectroscopy*, *ChemRxiv* **2026**, DOI: https://doi.org/10.26434/chemrxiv-2026-t8sfs.

Probing limits of PELDOR/DEER distance measurements

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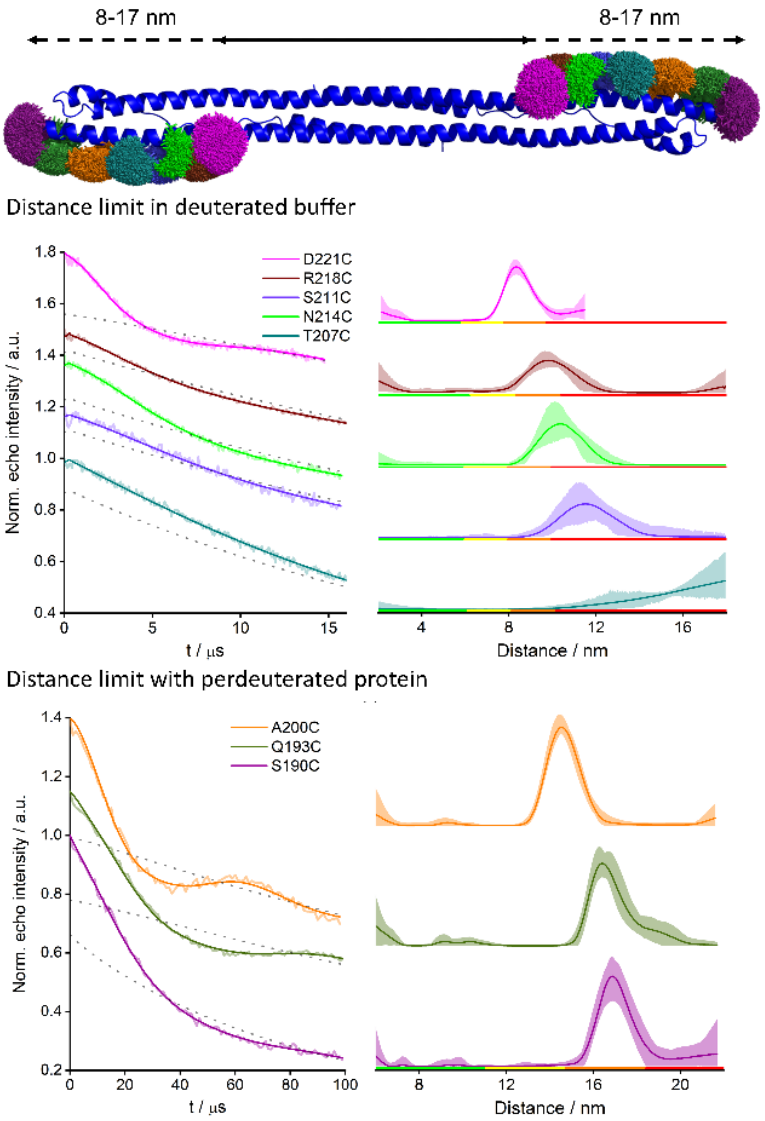
Pulsed dipolar electron paramagnetic resonance (EPR) spectroscopy (PDS) and in particular pulsed electron–electron double resonance (PELDOR/DEER), is a powerful method for determining nanometre-scale distances and distance distributions in biomolecular systems.

In this work, we explore PELDOR/DEER applications *in cellulo* identifying and testing different proteins and spin-labels for viability. However, recovery times after transfection pose the main challenge for applications in mammalian cells. Nevertheless, Cu-NTA combined with RIDME enables sensitive in-cell measurements and offers improved performance.



Investigating the long-range distance limits up to 10.5 nm could be reached under standard sample preparation conditions. By quantitative protein deuteration the accessible distance range is substantially extended, enabling accurate distance measurements up to 17.3 nm. Thereby exceeding the previously longest measured distance of 16 nm.[1] The sensitivity of the experiments was further enhanced through optimisation of the measurement and sample preparation conditions. Importantly, analysis of the achievable dipolar evolution times indicates that distances close to 20 nm should be experimentally accessible.

[1] Schmidt, *et al.*, *Angew. Chem. Int. Ed.* **2016**, *55*, 15905.

Abstracts - posters

Poster_01

Thiamine-Functionalized Maleated Chitosan: A Novel Bio-Based Adsorbent for Efficient Uptake of Methylene Blue from Aquatic Solutions

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Water contamination caused by synthetic pigments is a primary environmental concern, particularly in industries such as paper, plastics, and textiles, where large quantities of dyes are released into water sources [1-3]. However, excessive exposure to this dye can lead to adverse health effects, including skin and respiratory irritation, and in some cases, it may affect the nervous system and blood cells [4,5]. Removing methylene blue from water is crucial to preventing environmental and health hazards. Due to its strong chemical stability, this dye can persist in water sources, thereby reducing water quality and negatively impacting aquatic ecosystems.

In this study, a novel bio-based adsorbent, CSMA@TA, was successfully synthesized by grafting thiamine onto maleated chitosan (CSMA) and applied for the efficient removal of methylene blue (MB) from aqueous solutions. The composite was thoroughly characterized using FT-IR, SEM, TGA, XRD, and XPS, confirming successful functionalization and the presence of active binding sites. Batch adsorption experiments were conducted under varying conditions of solution pH (2–8), contact time (2–240 min), adsorbent dosage (0.01–0.05 g), initial dye concentration (25–250 mg/L), and temperature (298–318 K) to evaluate performance. Under optimal conditions (pH 8.0, 0.01 g adsorbent dose, 180 min contact time, 298 K, 100 rpm agitation), the CSMA@TA composite exhibited an exceptionally high maximum adsorption capacity of 230 mg/g, with a removal efficiency exceeding 93.4% at 25 mg/L MB concentration. The adsorption equilibrium was best described by the Langmuir isotherm model ($R^2 = 0.98555$), indicating monolayer adsorption on a homogeneous surface. The process followed pseudo-second-order kinetics ($R^2 = 0.98578$), suggesting that chemisorption governs the rate-limiting step. Thermodynamic analysis yielded negative Gibbs free energy values ($\Delta G°$ ranging from –24.85 to –23.56 kJ/mol), confirming the spontaneous nature of the process, while the negative enthalpy change ($\Delta H° = –44.08$ kJ/mol) indicated that adsorption was exothermic, accompanied by a decrease in entropy ($\Delta S° = –64.65$ J/mol·K). These results establish CSMA@TA as a sustainable, selective, and high-capacity adsorbent, demonstrating significant promise for wastewater dye remediation and broader environmental applications.

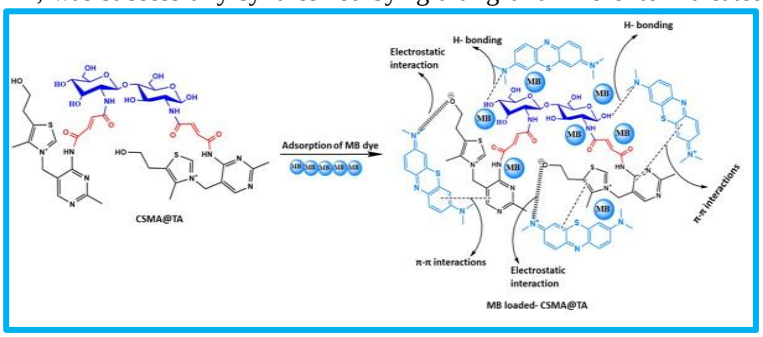

Figure 1. Proposed adsorption mechanism of methylene blue (MB) onto the CSMA@TA composite, illustrating the synergistic interactions including electrostatic attraction, π–π stacking, hydrogen bonding, and surface complexation that contribute to the high adsorption efficiency and stability of the material.

[1] Gaber, M., Shokry, H., Hassanin, A., Awad, S., Samy, M., & Elkady, M. Novel palm peat lignocellulosic adsorbent derived from agricultural residues for efficient methylene blue dye removal from textile wastewater. *Applied Water Science* **2025**, https://doi.org/10.1007/s13201-025-02363-y.

[2] Guven, M., Isik, B., Cakar, F., & Cankurtaran, O. Removal of toxic methylene blue dye from aqueous solutions by adsorption technique using magnetic loaded tea waste and its sodium alginate composite microspheres. *Environmental Monitoring and Assessment* **2025**, *197*(6), 664, https://doi.org/10.1007/s10661-025-14107-1.

[3] Samy, M., Tang, S., Zhang, Y., & Leung, D. Understanding the variations in degradation pathways and generated by-products of antibiotics in modified TiO2 and ZnO photodegradation systems: A comprehensive review. *Journal of environmental management* **2024**, *370*, 122402, https://doi.org/10.1016/j.jenvman.2024.122402.

[4] I.H. Alsohaimi, M.S. Alhumaimess, A.A. Alqadami, H.M.A. Hassan, Q. Chen, M.S. Alamri, M.M.J. Alanzi, T.S. Alraddadi, Chitosan-carboxylic acid grafted multifunctional magnetic nanocomposite as a novel adsorbent for effective removal of methylene blue dye from aqueous environment, *Chem Eng Sci.* **2023**, *280*, 119017, https://doi.org/https://doi.org/10.1016/j.ces.2023.119017.

[5] Kim, J., Jung, S., Kim, Y., Yoon, J., Kim, H., Jin, H. J., & Kwak, H. W. Eco-friendly Fish Gelatin Nanofibrous Membrane for Effective Cationic Dye Removal. *Surfaces and Interfaces* **2025**, 107096, https://doi.org/10.1016/j.surfin.2025.107096.

EPR Applications in Biomedical Science – from Structure Predictions to Native Proteins

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Here, we illustrate the power of EPR spectroscopy for biomolecular and biomedical applications, highlighting some of our recent research. Applications span from mechanosensitive channel under membrane tension[1] over cyclic nucleotide activated antiphage defence proteins[2,3] and riboswitches[4] to native metal ion binding sites in plasma proteins.[5,6]

[1] B. J. Lane, Y. Ma, N. Yan, B. Wang, K. Ackermann, T. K. Karamanos, B. E. Bode, C. Pliotas, Monitoring the Conformational Ensemble and Lipid Environment of a Mechanosensitive Channel Under Cyclodextrin-Induced Membrane Tension *Structure* **2024**, *32*, 739-750.

[2] S. McQuarrie, J. S. Athukoralage, S. A. McMahon, S. Graham, K. Ackermann, B. E. Bode, M. F. White, T. M. Gloster, Activation of Csm6 ribonuclease by cyclic nucleotide binding: in an emergency, twist to open *Nucleic Acids Res.* **2023**, *51*, 10590-10605.

[3] S. Gruschow, S. McQuarrie, K. Ackermann, S. A. McMahon, B. E. Bode, T. M. Gloster, M. F. White, CRISPR antiphage defence mediated by the cyclic nucleotide-binding membrane protein Csx23 *Nucleic Acids Res.* **2024**, *6*, 2761-2775.

[4] L. Remmel, A. Meyer, K. Ackermann, G. Hagelueken, M. Bennati, B. E. Bode, Pulsed EPR Methods in the Angstrom to Nanometre Scale Shed Light on the Conformational Flexibility of a Fluoride Riboswitch *Angew. Chem. Int. Ed.* **2024**, *63*, e202411241.

[5] K. Ackermann, S. Khazaipoul, J. L. Wort, A. I. S. Sobczak, H. EL Mkami, A. J. Stewart, B. E. Bode, Investigating Native Metal Ion Binding Sites in Mammalian Histidine-Rich Glycoprotein *J. Am. Chem. Soc.* **2023**, *145*, 8064–8072.

[6] K. Ackermann, D. Wu, A. J. Stewart, B. E. Bode, EPR spectroscopic characterisation of native Cu^{II}-binding sites in human serum albumin *Dalton Trans*. **2024**, *53*, 13529-13536.

Please go to S2_2

Poster_04

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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Web: https://www.chemistry.manchester.ac.uk/epr

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 (L-, 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 300 W Q-band amplifiers are available. Optical excitation spans the range from 210-2400 nm *via* tuneable OPO lasers of varying rep rate and power, simultaneous two-colour experiments are possible alongside a wide range of CW LEDs/lamps. We also possess loanable benchtop EPR spectrometers to enable on-site sample analyses with high throughput monitoring via variable temperature, auto sampler and (automated) goniometer accessories.

Support: The Facility can provide support for most experimental EPR techniques at multi-frequencies and variable temperatures; ranging from 1.8 K to 1000 K (frequency dependent) with cryogen-free cryostats and Liq. N_2 flow. 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.

Updates: Newly installed capabilities include: An additional 300 W Q pulse platform, Rapid-scan accessory (X-band), L-band pulse, Multi-harmonic detection (MHD) accessory. (HD100 for benchtop and floor standing platforms), Modernised electrochemical EPR apparatus and investment in high power and broad frequency range RF amplifiers for ENDOR (500 W to 250 MHz, 100 W to 1 GHz).

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 what EPR might do for your project**, please contact us for advice.

Poster_05

Differentiation of β-phosphorylated nitroxide diastereoisomers by complexation with cyclodextrins: an EPR study

Alexandru Gabriel Bucur[1], Sylvain Marque[1,2], Jean-Patrick Joly[1,2], Gabriela Ionita[1]

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

Host-guest chemistry of stable radicals has been extensively investigated for decades by electron paramagnetic resonance (EPR) spectroscopy. Most studies have focused on the inclusion complexation of nitroxides with cyclodextrins (CDs)[1], whereas significantly fewer reports address other type of radicals. Here, we examine the complexation of two diastereoisomers of a β-phosphorylated cyclic nitroxide radical with β-CD and γ-CD. Due to differences in the phosphorus and nitrogen hyperfine splitting constants, the two isomers display distinct EPR signatures. The cis stereoisomer (1c•) can form an intramolecular hydrogen bond between the hydroxyl group on the methylene substituent and an oxygen atom of the phosphoryl moiety; in contrast, this intramolecular interaction is not accessible for the trans stereoisomer (1t•). EPR spectra indicate a higher affinity of 1t• for γ-CD, evidenced by clear changes in the spectral parameters upon complex formation relative to the free radical. Binding constants derived from EPR data reveal stronger association with γ-CD than with β-CD, with the largest enhancement observed for 1t•. Moreover, increasing potassium chloride concentration enhances complex stability linearly by modulating solvation and electrostatic interactions, as confirmed by thermodynamic parameters obtained from EPR measurements. Overall, these results underscore the decisive roles of molecular stereochemistry and ionic strength in governing cyclodextrin-nitroxide host-guest interactions.

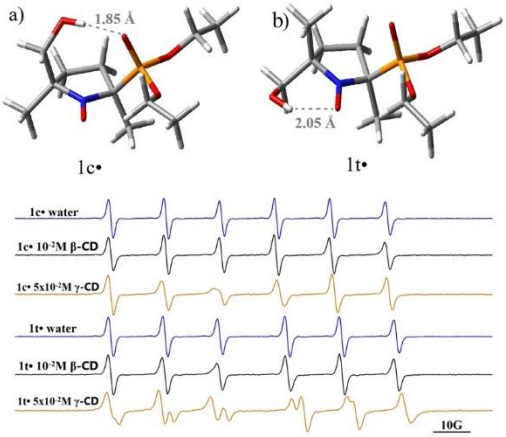

Figure 1. Geometries of 1c• (a) and 1t• (b) obtained with DFT calculations and the EPR spectras of the two radicals in water and CD solutions.

[1] E. G. Bagryanskaya and S. R. A. Marque, in Electron Paramagnetic Resonance, *ed*. V. Chechik and D. M. Murphy, *Royal Society of Chemistry* **2017**, *25*, 180–235, DOI: 10.1039/9781782629436.

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.

Poster_06

Molecular Alignment and Quantum State Tomography for Assessing Gate Fidelity in Molecular Electron Spin Qubits

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EPSRC National Research Facility for Electron Paramagnetic Resonance, Department of Chemistry and Photon Science Institute, University of Manchester, Oxford Road, M13 9PL, UK.

For decades, quantum technology has promised vast improvements in the amount of computational power and time required to carry out calculations for which quantum algorithms can be found. These include applications such as cryptography (Shor's algorithm), database searching (Grover's algorithm) and simulation of chemical processes.[1] However, implementing such systems has proven a challenge, with many different approaches proposed, such as quantum dots, trapped ions and superconductors.[2] The work carried out aims to contribute to the implementation of Molecular Electron Spin Qubits (MESQs) as a candidate system for quantum computation.

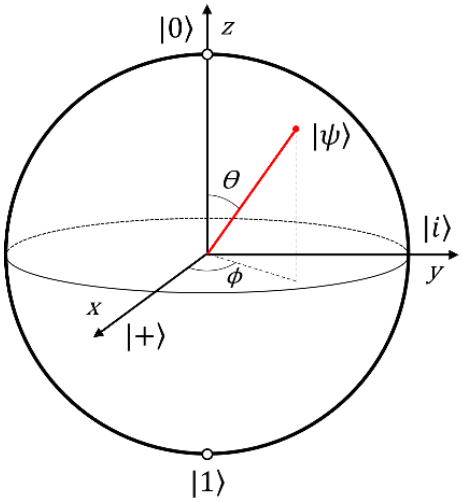

Figure 4: The Bloch sphere representation of a single qubit. Polar coordinates describe the qubit state as a vector on a unit sphere.

MESQs employ the two spin states of an unpaired electron, which can be controlled using microwave pulses, and measured by EPR spectroscopy. Previous research has suggested that molecular alignment of candidate systems should improve quantum gate fidelities.[3] In this work we explore the use of liquid crystals to align molecules and characterize the impact of restricted molecular orientations as a result of the alignment matrix on the distribution of dipolar frequencies measured by orientationally-selective Double Electron-Electron Resonance (DEER) compared to disordered frozen solution samples.[4]

[1] D. P. Divincenzo, *Fortschr. Phys*. **2000**, *48*, 771-783.
[2] H. A. Bhat, F. A. Khanday, *et al*., *IEEE Open Journal of Nanotechnology* **2022**, *3*, 61-77.
[3] E. J. Little, J. Mrozek, C. J. Rogers, *et al*., *Nat Commun* **2023**, *14*, 7029.
[4] J. E. Lovett, A. M. Bowen, *et al*., *Phys. Chem. Chem. Phys.* **2009**, *11*, 6840-6848.

Poster_07

High-Field EPR Spectroelectrochemistry – Development and Application

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Department of Physical Chemistry, University of Stuttgart, Germany

Inspired by cofactors, modern catalysts often feature transition metal centers,[1] whose redox processes can be probed by cyclic voltammetry[2] and characterized by EPR spectroscopy.[3] For integer spin species, high-field EPR is essential to access transitions silent at X-band (9.5 GHz).[3] Integer-spin species such as chromium(II), manganese (III) are highly relevant for 3d transition metal catalysis. To enable *in situ* and *operando* studies under these conditions, we present a high-field EPR spectroelectrochemical (HFEPR-SEC) cell operable between 180 and 360 GHz.

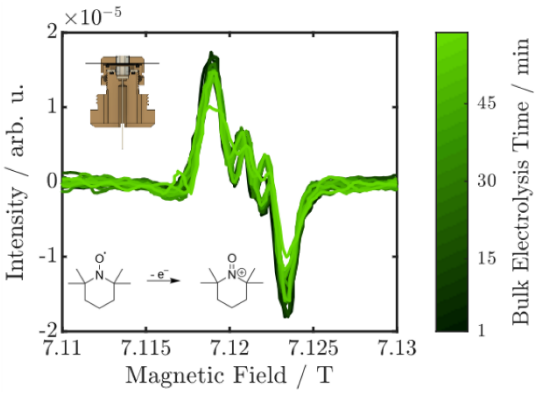

Figure 1. HFEPR spectra of TEMPO measured at room temperature and 200 GHz during continuous electrochemical TEMPO-oxidation.

We present the development of an HFEPR sample holder compatible with both high-field EPR measurements and electrochemical experiments. Unlike conventional EPR, high-field EPR operates without a resonator,[3] necessitating a fundamentally different sample holder geometry. In our design, the working electrode serves a dual function as both electrode and microwave mirror. The custom three-electrode setup behaves as a Randles circuit, as confirmed by Electrochemical Impedance Spectroscopy. High-quality cyclic voltammograms of various transition metal complexes were successfully recorded. Successful HFEPR measurements were per-formed on TEMPO at room temperature and in frozen solution, as well as on transition metal complex solutions at cryogenic temperatures. As a proof of concept, *in situ* EPR measurements were conducted during the bulk electrolysis of TEMPO at room temperature. The oxidation process could be monitored spectroscopically, as evidenced by a decrease in signal intensity corresponding to the loss of the paramagnetic species.

As a new method, HFEPR-SEC enables the investigation of catalysts and their reactive intermediates during catalytic reactions. By combining electrochemistry with high-field EPR, it allows *in situ* characterization of paramagnetic species, including those of integer spin. This approach offers powerful new opportunities for mechanistic studies by providing valuable insights into electronic structure changes during catalytic reactions.

[1] E. G. Samsel, K. Srinivasan, J. K. Kochi, *J. Am. Chem. Soc.* **1985**, *107*, 7606–7617.

[2] N. Bhuvanendran, S. Ravichandran, Q. Xu, T. Maiyalagan, H. Su, *Int. J. Hydrog. Energy* **2022**, *47*, 7113–7138.

[3] P. Neugebauer, J. van Slageren, *Phys. Chem. Chem. Phys.* **2018**, *20*, 15528–15534.

Coherent Manipulation of Organometallic Ti (III) and Hf (III) Molecular Spin Qubits

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[b]*Department of Chemistry, University of Rhode Island, RI 02881, USA.*

The advancement of quantum information science relies on the realization of robust qubits with long coherence times[1]. Since spin–orbit coupling (SOC) often accelerates decoherence, mitigating the influence of SOC has become an effective strategy for extending coherence times. Herein, two S = ½ group 4 molecular systems have been researched by cw-EPR and pulsed-EPR, considering that pseudo-*C*3 symmetry could enable the unpaired electron in the d_z^2 orbital[2], which also permit the orbital mixing with s orbital[3].

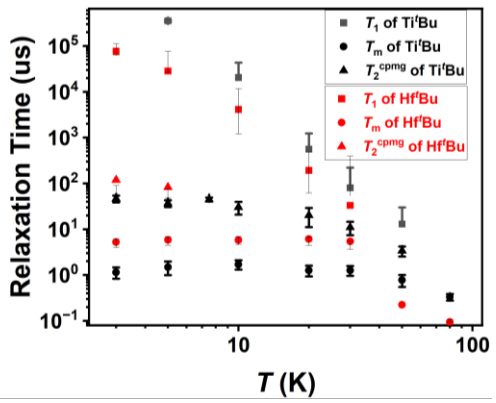

Figure 1. Temperature dependence of T_1, T_m, T_2^{cpmg} for Ti^{t}Bu and Hf^{t}Bu at OP2.

Herein, thermally stable examples of $Hf^{III}(OAr^R)_3$ (OAr^R = OC_6H_3-2,6-^{t}Bu-4-R; R = H, ^{t}Bu) complexes were isolated by chemical reduction of $BrHf(OAr^R)_3$ precursors using KC_8. These Hf^{III} complexes adopt a trigonal planar geometry and DFT calculations best describe their SOMO as a mixed *s*-d_z^2 orbital character with 32% *s*-orbital character. We report the first examples of resolved hyperfine coupling to ^{177,179}Hf (^{177}Hf, I = 7/2; ^{179}Hf, I = 9/2) in a molecular Hf^{III} complex, with X-band CW EPR revealing the largest hyperfine interactions of A_x = 1320 MHz, A_y = 1360 MHz and A_z = 1325 MHz for ^{177}Hf (I = 7/2) and A_x = 829 MHz, A_y = 854 MHz and A_z = 832 MHz for ^{179}Hf (I = 9/2). Long spin-lattice relaxation times (T_1) of 123.2 ms were observed, and dephasing times have been observed using a Carr-Purcell-Meiboom-Gill sequence, reaching 118 µs at 3 K. Comparisons between Ti^{III}, Zr^{III}, and Hf^{III} supported by the same ligand scaffold are de-scribed show that the phase memory time increases with increasing metal *s*-orbital character in the SOMO. This study introduces Hf^{III} ions as competitive molecular qubits and expands the scope of useful metal ions to include more earth-abundant metals.

[1] Wedge, *et al*., *Phys. Rev. Lett*. **2012**, *108*(10), 107204.
[2] Ariciu, *et al*., *Nat. Commun.* **2019**, *10*(1), 3330.
[3] Nodaraki, *et al*., *J. Am. Chem. Soc*. **2024**, *146*(22), 15000-15009.

Poster_09

A Topologically Frustrated Non-Kekulé Nanographene as a Molecular Qubit

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Carbon-based non-Kekulé molecular systems with intrinsic spin represent a promising route toward qubit operation at ambient temperatures. In particular, topologically frustrated nanographenes offer a unique molecular platform for engineering correlated and entangled spin states. However, experimental exploration of these systems has been severely constrained by the scarcity of viable molecular topologies, demanding synthetic routes, and limited structural stability1,2

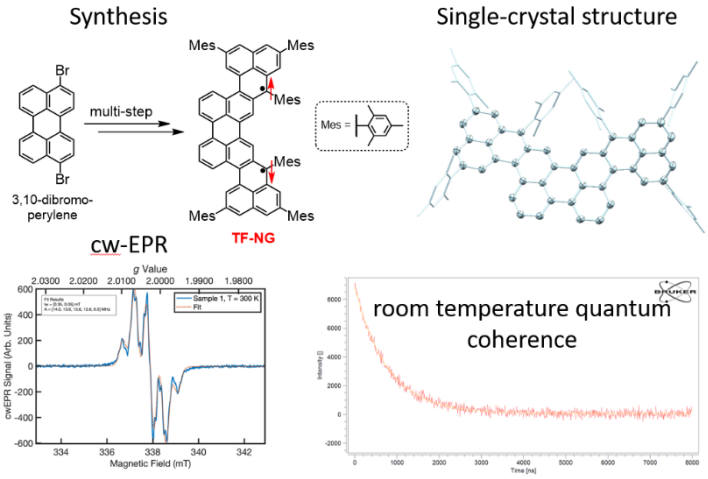

Figure 1. Solution synthesis, single crystal structure, cw-EPR and room temperature quantum coherence in a topologically frustrated nanographene.

Here, we report the solution synthesis and isolation of a topologically frustrated nanographene featuring a concealed non-Kekulé structure that hosts two antiferromagnetically coupled spins. A symmetric molecular design, combined with kinetic stabilization of the high-spin sites, enables crystallization of this otherwise elusive open-shell system, with its structure unambiguously confirmed by single-crystal X-ray diffraction (XRD). Electron paramagnetic resonance (EPR) spectroscopy reveals antiferromagnetic exchange coupling and establishes the entangled nature of the two spins. Remarkably, the resulting entangled spin pair functions as a molecular qubit system, exhibiting long spin-coherence times on the order of microseconds even at room temperature. These results provide direct experimental evidence of spin entanglement and coherent quantum behavior in a topologically frustrated nanographene, positioning such systems as promising molecular candidates for future quantum technologies.

[1] Lombardi, F., *et al.*, *Science* **2019**, *366*, 1107–1110.
[2] Lombardi, F., *et al.*, *Chem* **2021**, *7*, 1363–1378.
[3] Jiao, T., *et al.*, *Nat. Chem*. **2025**, *17*, 924–932.

Photonic Band-Gap Resonators Design for High-Field Electron Paramagnetic Resonance

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High-field Electron Paramagnetic Resonance (EPR) spectroscopy (≥7 T, ≥200 GHz) provides enhanced sensitivity and g-tensor resolution, and reduced spectral congestion compared to conventional low-field EPR. However, the broader application of high- field EPR remains constrained by the limited availability of mm-wave power and is often exacerbated by the use of non-resonant setups, further limiting the available mm-wave (mmW) magnetic fields (B_1).

Resonant structures can enhance the B_1 at the sample, thereby improving sensitivity under power-limited conditions. Photonic band-gap resonators (PBGRs) offer a scalable solution for enhancing the mmW B_1 at high frequencies. These resonators are formed by introducing lattice defects into periodic structures composed of low-loss dielectric materials[1], enabling strong confinement of mm-wave radiation (inset in Fig. 1A). By positioning the sample at a magnetic-field maximum and an electric-field node, PBGRs minimize dielec- tric losses while supporting larger sample volumes than single-mode resonators.

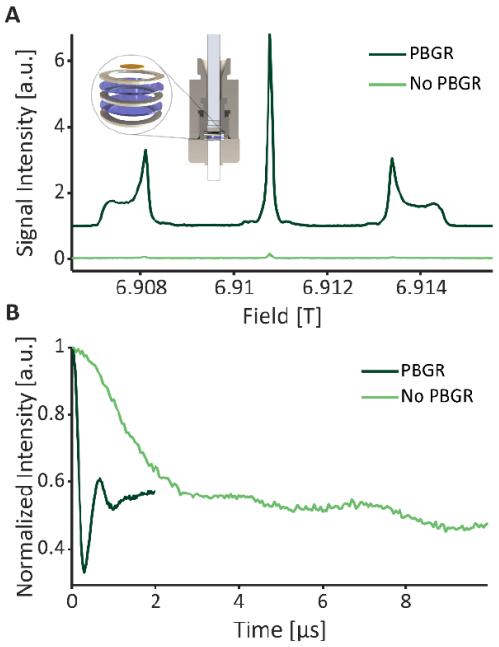

Figure 1. A Comparison of a pulsed EPR field sweep of P1 centers in a CVD diamond with and without PBGR, at 194 GHz. **B** Comparison of a 3-pulse nutation at of 1% w/w BDPA in PS with PBGR and of P1 centers in a diamond without PBGR, at 388 GHz.

Here, we report the design, optimization, and experimental performance of PBGR at 7 T (194 GHz) and 14 T (388 GHz) implemented on a home-built high-field EPR spectrometer[2]. At 7 T (194 GHz), we demonstrate 750-fold signal enhancement for BDPA and 43-fold improvement in SNRs for CVD diamond (Fig. 1A) at 10 K and room temperatures (RT). For the 14 T (388 GHz) implementation, we achieved a 10-fold enhancement in B1 relative to a non-resonant configuration (Fig. 1B) in RT experiments.

[1] S. Milikisiyants, A. A. Nevzorov, and A. I. Smirnov, *JMR* **2018**, *296*, 152-164.

[2] O. Nir-Arad, D. H. Shlomi, A. Israelstam, T. Amit, N. Manukovsky, A. B. Fialkov, and I. Kaminker. *JMR* **2024**, *360*, 107635.

Please go to S3_2

ENDOR study of the electronic structure of chemically oxidised copper(II) porphyrins

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Porphyrins offer a customisable scaffold for the engineering of molecular devices such as qubits or quantum sensors[1]. The electronic properties of porphyrins can be tuned both by choice of metal and by choice of substituents. Furthermore, porphyrins can be assembled into supramolecular architectures which exhibit interesting properties such as electronic delocalisation in the ground and excited state, spin polarisation, and global aromaticity/anti-aromaticity.[2-3] The incorporation of paramagnetic metals at the centre of porphyrins allows for the investigation of high spin molecular complexes which are of interest as potential qudits, utilising their higher dimensional Hilbert spaces to increase the density of quantum information that can be stored and manipulated.

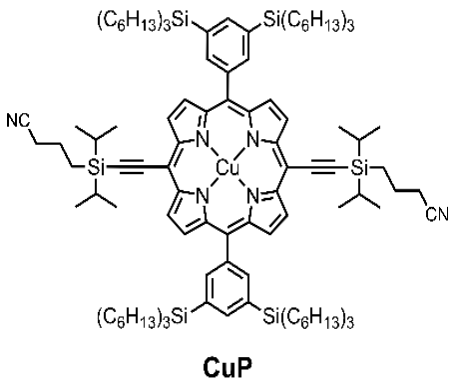

Figure 1. Structure of the copper(II) porphyrin investigated in this work.

In this work, we employ various pulsed ESR experiments and simulations to characterise the triplet spin state of the cation of the copper porphyrin **CuP** (Figure 1). We provide explicit evidence for a triplet state *via* hyperfine-correlated ^{1}H-Mims ENDOR and field-swept ^{14}N-Davies ENDOR. We use simulations to quantify the g-factor and zero-field splitting of the cationic state. Finally, we propose an ENDOR experiment for assigning the absolute sign of the hyperfine and zero-field splitting tensors for thermally accessible triplet states, where single crystal or temperature dependent studies are difficult or impossible.

A detailed characterisation of the rich spin Hamiltonian of the seemingly simple **CuP**$^{+}$ system is vital for understanding the electronic properties of more complex copper(II) porphyrin oligomer systems. This work lays the foundations for future studies of copper(II) dimers in the chemically oxidised state whereby the removal of a porphyrin π-electron may lead to modulation of the exchange coupling between the metals.

[1] F. Santanni, A. Privitera, Metalloporphyrins as Building Blocks for Quantum Information Science. *Adv. Optical Mater.* **2024**, *12*, 2303036.

[2] Peeks, M., Claridge, T. & Anderson, H. Aromatic and antiaromatic ring currents in a molecular nanoring. *Nature* **2017**, *541*, 200–203.

[3] J. Hergenhahn, S.M. Kopp, H. Gotfredsen, K. Tang, S. Barlow, S.R. Marder, C.R. Timmel, H.L. Anderson, *Angew. Chem. Int. Ed.* **2025**, *64*, e202518425.

Multiphoton Double Electron Electron Resonance

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Department of Chemistry, University of Manchester, Oxford Road M13 9PL Manchester, United Kingdom.

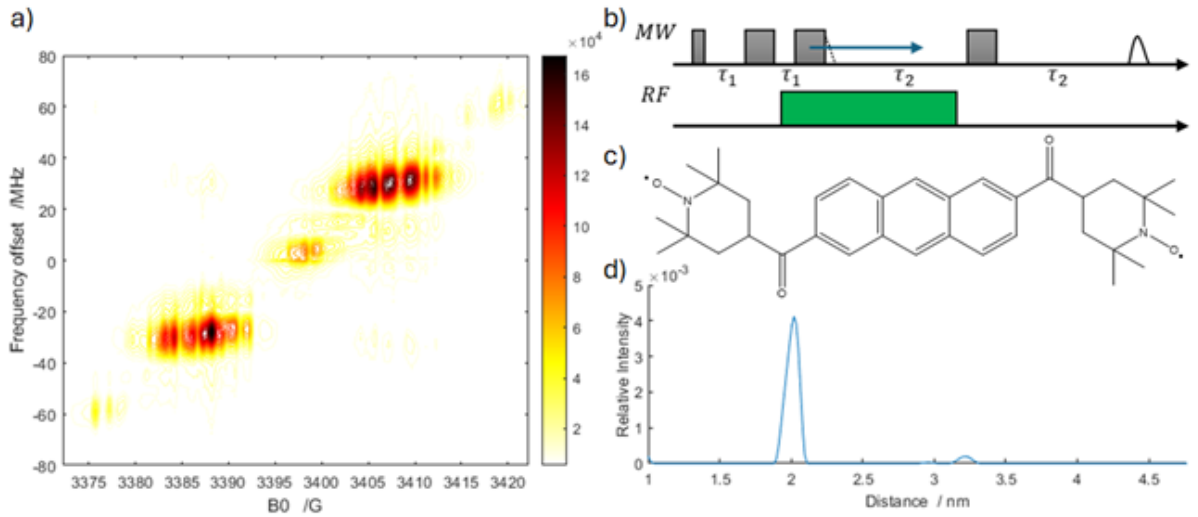

Figure 1. a) Multiphoton transitions observed for a Hahn echo with simultaneous mw and rf pulses on coal. b) Multiphoton DEER pulse sequence. c) A nitroxide biradical, for which d) shows the distance distribution obtained following a multiphoton DEER experiment.

Transitions between spin states can be achieved by a combination of photons. These multiphoton transitions pass through virtual states and can be described by Floquet theory [1]. For a spectrometer setup which simultaneously uses microwave (mw) and radiofrequency (rf) sources, resonances can be observed at frequencies of ω_{mw}, $\omega_{mw} \pm \omega_{rf}$, $\omega_{mw} \pm 2\omega_{rf}$ etc. The transition probabilities for the various resonances can be manipulated with the choice of rf power and rf frequency used, and the ω_{mw} resonance can be made to disappear entirely, in a 'π-photon-induced-transparency' condition [2], [3]. This project demonstrates the use of the 'π-photon-induced-transparency' condition in a multiphoton version of the Double Electron Electron Resonance (DEER) experiment. The 4-pulse DEER sequence usually requires the 3rd pulse, acting on 'pump' spins to have a distinct mw frequency from all other pulses, acting on 'detect' spins. In multiphoton DEER, the 3rd pulse is at the same mw frequency, but also includes an rf component which satisfies the 'π-photon-induced-transparency' condition. So, only the various multiphoton transitions are involved during the 3rd pulse, and the requirement for a distinct frequency is effectively satisfied. Multiphoton DEER is demonstrated (Fig 1.), and its advantages discussed.

This work was supported by the Royal Society.

[1] Ivanov, K.L., *et al*, *Progress in NMR Spectroscopy* **2021**, *126-127*, 17-582.

[2] Fedin, M., *et al*., *The Journal of Chemical Physics* **2004**, *120*(3), 1361-1368.

[3] Kälin, M., ETH Zürich, Nr. 15142, **2003**. https://doi.org/10.3929/ethz-a-004593146.

Poster_14

Spin communication in TTM-based chromophore—radical systems

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Tris(tricholorphenyl)methyl (TTM) radicals possess high stabilities, owing to electronic and steric effects, as well as narrow EPR lines and long coherence times, relative to nitroxide-based radicals. Functionalisation of TTM radicals with electron-donating groups, such as carbazole, render these radicals highly fluorescent [1]. Incorporated within chromophore–radical dyads these systems allow optical initialisation of spin–spin interactions and the inherent modularity enables systematic modifications (chromophore type, distance, or orientation) toward tailored properties in applications such as electron-spin hyperpolarisation, photochemical up-conversion and spin-optical interfaces for QIS [2–5].

In this contribution we explore a series of TTM-based chromophore–radical systems, investigating how the chromophore substitution position and energetics influence the excited state dynamics and properties. Across the series we show the yields and lifetimes of excited state processes are sensitive to small energetic changes and demonstrate the formation of quartet states with differing spin-polarisation and relaxation properties. The results clearly emphasise the need to consider triplet and charge transfer state energies as well as chromophore substitution positions for an optimised molecular design.

[1] Gamero, V.; Velasco, D.; Latorre, S.; López-Calahorra, F.; Brillas, E.; Julía, L. *Tetrahedron Lett.* **2006**, *47*, 2305–2309, 10.1016/j.tetlet.2006.02.022.
[2] Yabuki, R.; Nishimura, K.; Sawada, Y.; Fuki, M.; Kobori, Y.; Yanai, N. *J. Magn. Reson. Open* **2025**, *22*, 100181, 10.1016/j.jmro.2024.100181.
[3] Richards, K. D.; Wang, W.; Thielert, P.; Green, J.; Hudson, J.; Tonnelé, C.; Casanova, D.; Olivier, Y.; Hele, T.; Richert, S.; Li, F.; Evans, E. W. *ChemRxiv* **2024**, 10.26434/chemrxiv-2024-2gf9b.
[4] Gorgon, S., Lv, K., Grüne, J., *et al.*, *Nature* **2023**, *620*, 538–544, 10.1038/s41586-023-06222-1.
[5] Chen, Y.; Palmer, J. R.; Phelan, B. T.; Peinkofer, K. R.; Krzyaniak, M. D.; Young, R. M.; Wasielewski, M. R., *J. Am. Chem. Soc.* **2025**, *147*, 42, 38762–38771, 10.1021/jacs.5c14244.

Poster_15

Tuning the Zero-Field Splitting of Ni(II)-based Complexes for on-Chip Superconducting Kinetic Inductance Readout

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Molecular Qubits (MQBs) exploit the electronic spin in molecules to access quantum properties, and are investigated towards applications such as quantum computing, quantum sensing, or quantum communication.[1] An interesting case is when such systems have more than two spin levels that can be addressed and manipulated individually. These systems, called Molecular Qudits (MQs), can be based on the hyperfine levels[2] or on multi-spin levels (S=1 or more).[3] However, most of these systems are EPR-silent because they do not show any transition at EPR frequencies that are typical for commercial spectrometers (9 and 35 GHz). In order to investigate MQs it is important to develop new methodologies that allow studying the spin properties of MQs in a broad frequency range. Here, we aim to investigate superconduct- ing on-chip kinetic inductivity detectors (KIDs) to readout the EPR signal of MQs (Figure 1). In principle, these resonators can work at every frequency, can be multiplexed, and their sensitivity can reach the single photon level.[4] Within the project we will design, fabricate and characterize KID resonators, which will then be applied to investigate a series of S=1 MQs.

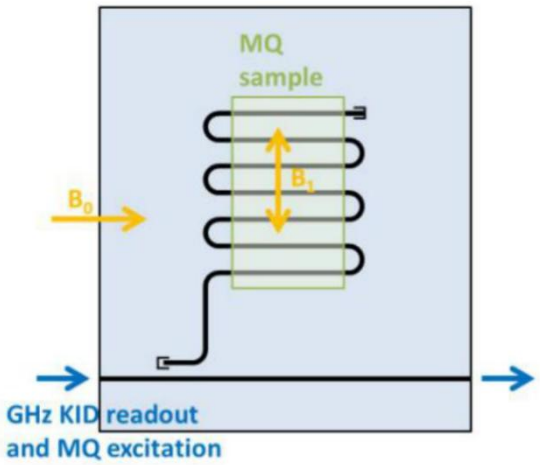

Figure 1. Scheme of the setup of a resonator on a KID with an MQ sample.

In this specific contribution, I will show first characterization of the KID resonators using S=1/2 molecules like TEMPOL and $Cu(acac)_2$. Additionally, I will present the synthesis of a series of Ni(II) octahedral complexes with engineered zero-field splitting gaps[5] and their characterization by SQUID magnetometry, as well as X-band and High Frequency EPR spectroscopy.

[1] L. Tesi, *et al.*, *Chem. Sci.*, **2016**, *7*, 2074-2083.
[2] S. Carretta, *et al.*, *Chem. Sci.*, **2021**, *12*, 12046-12055.
[3] T. Mallah, *et al.*, *J. Am. Chem. Soc.* **2025**, *147*, 4685-4688.
[4] G. Ulbricht, *et al.*, *Appl. Sci.* **2021**, *11*, 2671.
[5] J. Titis and R. Boca, *Inorg. Chem.* **2010**, *49*, 3971-3973.

Harnessing fluorescent labels for novel in-cell biological structural determination using magnetic resonance

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a) The National Research Facility or Electron Paramagnetic Resonance, Department of Chemistry and Photon Science Institute, The University of Manchester.
b) Department of Chemistry, Manchester Institute of Biotechnology, The University of Manchester.
c) BioEmPiRe Centre for Structural Biological EPR Spectroscopy, School of Biological Sciences, Faculty of Biology, Medicine and Health, University of Manchester, Manchester, United Kingdom
d) Department of Chemistry, School of Natural Sciences, The University of Manchester, Oxford Road, Manchester, UK

Non canonical amino acids (NCAA) are driving forward synthetic biological proteins allowing mechanisms that previously were impossible. One application is in an enantioselective [2 + 2] cyclase through triplet energy transfer in a protein called VEnT. VEnT contains a NCAA of thioxanthone (Figure 1) that facilitates this reaction.[1] Here, we employ this NCAA for Electron Paramagnetic Spectroscopy (EPR) functions within VEnT to investigate its properties as a photoswitchable triplet-state spin-label. We show that the triplet signal obtained is detectable via both trEPR (time resolved EPR) methodologies and pulsed EPR, and that the measured relaxation times are favourable for the application of light- induced EPR pulse dipolar spectroscopy (PDS) methods such as light induced double electron-electron resonance (LiDEER)[2] and laser induce magnetic dipoles (LaserIMD)[3]. The use of a triplet-state NCAA spin-label widens the opportunities for available orthogonal spin-labelling and could have potential applications for in-cell EPR.

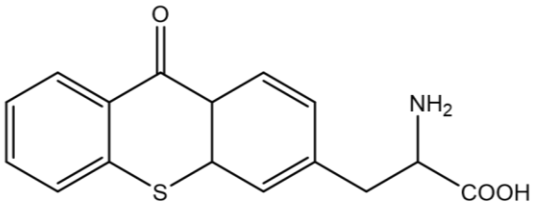

Figure 1: Thioxanthone based non canonical amino acid.

[1] Trimble, J.S., Crawshaw, R., Hardy, F.J., *et al.*, A designed photoenzyme for enantioselective [2+2] cycloadditions. *Nature* **2022**, *611*, 709–714.

[2] Di Valentin, M.; Albertini, M.; Zurlo, E.; Gobbo, M.; Carbonera, D.; Porphyrin Triplet State as a Potential Spin Label for Nanometer Distance Measurements by PELDOR Spectroscopy. *J. Am. Chem. Soc.* **2014**, *136* (18), 6582–6585.

[3] Hintze, C.; Bücker, D.; Domingo Köhler, S.; Jeschke, G.; Drescher, M.; Laser-Induced Magnetic Dipole Spectroscopy. *J. Phys. Chem. Lett.* **2016**, *7* (12), 2204–2209.

Electronic Structure of Lanthanocene and Actinocene $[Ln/An(COT)_2]^n$ Complexes

Iulia Turcas[1,2], Cameron N. Deakin[1,3], Benjamin L. L. Réant[1,3], Liam P. Griffin[1,3], Adam Brookfield[2], David Collison[1,2], Conrad A. P. Goodwin[1,3] and Eric J. L. McInnes[1,2]

[1]*Department of Chemistry, The University of Manchester, Manchester, UK.*
[2]*Photon Science Institute, The University of Manchester, Manchester, UK.*
[3]*Centre for Radiochemistry Research, The University of Manchester, Manchester, UK.*

Understanding actinide electronic structure holds great interest for applications in nuclear-fuel reprocessing, civil nuclear-waste management and nuclear forensics [1]. However, compared to 4*f* valence metal ions, 5*f* systems exhibit enhanced relativistic and ligand field effects, leading to often difficult-to-rationalize electronic structures and bonding properties [2].

Here, we investigate a series of lanthanocene and actinocene complexes in which the central metal ion is sandwiched between two cyclooctatetraene (COT^{2-}) dianions using electron paramagnetic resonance (EPR) spectroscopy. Continuous-wave X-band EPR and variable-temperature SQUID magnetometry were used to characterize the nature of the electronic ground states of a redox family of $[Ln/An(COT)_2]^n$ (*n* = charge) complexes and substituted analogues (**Figure 1**). The EPR and magnetic data are interpreted to assign the ground spin-orbit states and are discussed in the context of the electronic structures.

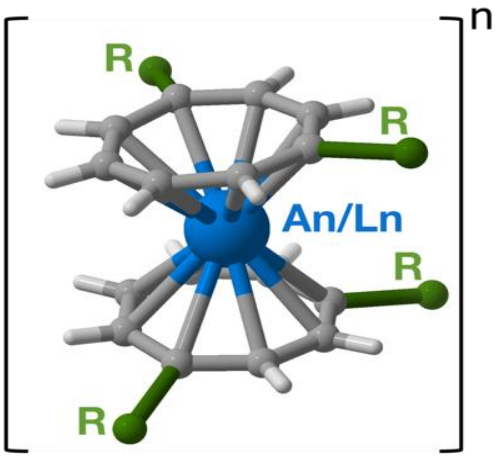

Figure 1. Molecular structure of actinocene and lanthanocene $[Ln/An(COT)_2]^n$ complexes.

Through this work, we highlight the need for systematic studies across broader families of actinide compounds to gain a clearer understanding of *f*-element chemistry and to improve the accuracy of quantum-chemical models.

[1] K. T. Moore, C. A. Marianetti and G. H. Lander, *MRS Bull.*, **2010**, *35*, 841–847.
[2] F. Gendron and J. Autschbach, *Encycl. Inorg. Bioinorg. Chem.*, **2018**, 59–76.

Poster_18

EPR Study on the Interaction of Oxygen and Nitric Oxide with Octa-Substituted Cobalt Phthalocyanines

Runyu Zhang[1], Yuxiang Zhang,[1] Shannah Kerrigan,[2] Neil McKeown,[2] Floriana Tuna[1]

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Following the successful crystallization of nanoporous crystals of cobalt(II) phthalocyanine complexes of formula [(dipPhO)8PcCo] (**PcCo**) (dipPhO = di-isopropyl-phenoxy), and related dimeric systems, **PcCo-bipy-CoPc** and **PcCo-bpm-CoPc** (bipy = 4.4'-bipyridine; bpm = 4,4'-bipyrimidine)[1], followed by *in-situ* X-ray crystallography observation of NO and CO binding at the Co site within the voids of phthalocyanine nanoporous crystals (PNCs)[2], an electron paramagnetic resonance (EPR) spectroscopy study was initiated to study the systems before and after NO gas sorption, aiming to understand their NO binding ability and any transformations that occur during these reactions. During the project the investigation was expanded to also probe the binding of O_2, given the relevance of these systems as synthetic models for cobalamin or hemes.

The studies included a set of powder, solution and single crystal EPR experiments conducted over the temperature range 5-80 K. Resulted spectra have been simulated to provide consistent magnetic parameters that helped identify the compounds and probe their environments and oxidation states. The studies found that O_2 binds reversibly and selectively in all these compounds, leading to the formation of a Co-$O_2^{\bullet-}$ species irrespective of the status of the material. In contrast, NO sorption into solid samples (single crystals or powdered crystals) led to irreversible formation of **CoPc(NO)** adducts, along with a new radical species whose origin could not be unambiguously established. The whole *in-situ* NO gas adsorption process on cobalt ions was well captured by CW EPR, unbound NO molecules were present at 80 K by probing the NO gas that has a very characteristic g≈0.78 value.

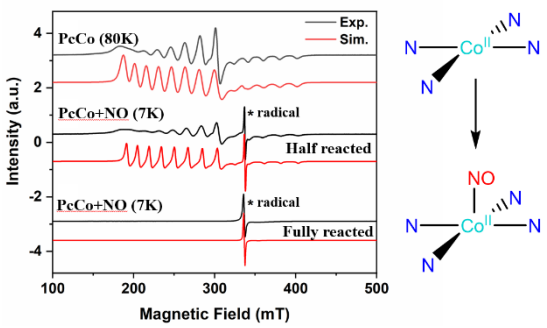

Figure 1. EPR spectra of **PcCo** under NO gas adsorption.

[1] C. Grazia Bezzu, B. M. Kariuki, M. Helliwell, F. Tuna, J. E. Warren, D. R. Alland and N. B. McKeown, *CrystEngComm* **2013**, *15*, 1545-1550.

[2] N. Stamos, C. J. McMonagle, G. F. Turner, D. R. Allan, M. R. Warren, A. J. Warren, N. B. McKeown and S. A. Moggach, *Chem. Commun.* **2024**, *60*, 1150811511.

Poster_19

Measuring Spin Relaxation Times by Pulsed EPR for Nitrogen Dioxide Loaded in Metal-Organic Frameworks

Yuxiang Zhu[1,2], Martin Schröder*, Sihai Yang* and Floriana Tuna*

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Nitrogen dioxide (NO_2) is a toxic pollutant that causes enormous environmental and health problems. Monomeric NO_2 is a radical gas with a single electron mainly localized on the nitrogen atom. This allows to use electron paramagnetic resonance (EPR) methods to probe the status of NO_2 loaded into porous materials such as metal-organic frameworks (MOFs).

Herein we use pulsed EPR to measure the spin-lattice relaxation time, T_1, and spin -spin relaxation time, T_2, for NO_2 molecules adsorbed into MIL-96(Al) and MFM-520(Zn) MOFs and under different pressures, to gain understanding of host–guest interactions occurring between NO_2 and MOF surface, and the guest-guest interactions occuring between neighbouring NO_2 molecules.

This work will encourage the methods of designing MOFs for challenging gas adsorption and expands usage of EPR spectroscopy to analyzing interaction of guest molecules in porous materials.

[1] J. Li, X. Han, X. Zhang, A. M. Sheveleva, Y. Cheng, F. Tuna, E. J. L. McInnes, L. J. McCormick McPherson, S. J. Teat, L. L. Daemen, A. J. Ramirez-Cuesta, M. Schroder and S. Yang, *Nat Chem* **2019**, *11*, 1085-1090.

Intermolecular spin coupling in binary chromophore–radical systems

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In the field of dynamic nuclear polarisation solutions with high radical concentrations (> 20 mM) are often used. Despite these high concentrations, dipolar coupling is assumed to be dominant because only intermolecular interactions are involved.[1] Thus far it remains unclear to which extent the exchange coupling, characterised by the exchange coupling parameter *J*, plays a role in intermolecular spin–spin interactions.

Assemblies consisting of a chromophore C, a linker and a radical R, are excellent model systems to investigate spin–spin interactions, coupling regimes and high-spin states.[2] Upon light excitation, a triplet state at the chromophore unit is generated which may interact with the stable organic radical. A variety of studies investigate covalently–bound C–R dyads demonstrating the tunability of *J*.[2] Recently it was also shown, that the strong coupling regime can be reached in supramolecular assemblies, more precisely for a chromophore unit linked to a radical unit via three hydrogen bonds.[3]

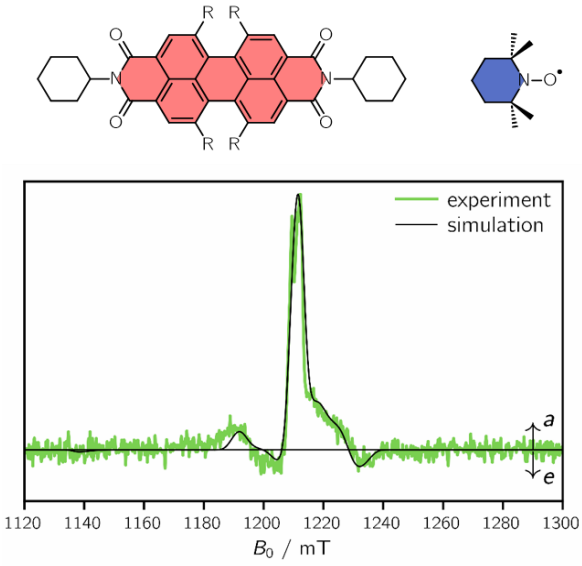

Figure 1. The investigated chromophore (PDI) and radical (TEMPO) and experimental trEPR data of a binary solution with 1:200 chromophore to radical ratio along with its EasySpin[4] simulation.

This work investigates intermolecular spin–spin interactions and shows, that the ex- change interaction *J* remains pertinent to intermolecular considerations, even in the absence of specific intermolecular interactions such as hydrogen bonding or covalent linkage. Transient continuous wave EPR (trEPR) experiments suggest that high spin (quartet) states can be formed in a binary system consisting of the chromophore PDI and the radical TEMPO, indicating strong exchange coupling between the two units.

[1] Denysenkov, V; Prisner, T *eMagRes* **2019**, *8*, 41–54.
[2] Quintes, T.; Mayländer, M.; Richert, S. *Nat. Rev. Chem.* **2023**, *7*, 75–90.
[3] Khariushin, I. V.; Thielert, P.; Mayländer, M.; Zöllner, E.; Quintes, T.; Richert, S.; Vargas Jentzsch, A. *Nat. Chem.* **2025**, *17*, 493–499.
[4] Stoll, S.; Schweiger, A. *J. Magn. Reson.* **2006**, *178*, 42–55.

Kestrel: A ligand-field program to probe the spectroscopy of 3d transition metals in real-time

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Kestrel is a computational package that performs ligand field calculations on any 3d transition metal complex in any coordination geometry. It has been applied to investigating d-d transitions in Fe(IV)-oxido species [1] and spin-crossover in Fe(II) complexes [2]. Kestrel computes d-d transition energies, paramagnetic susceptibilities and EPR g-factors and hyperfine values.

Kestrel assumes minimal spatial overlap between the metal and ligand orbitals, however it calculates the two-electron integral for dynamical correlation between d-orbital configurations brought about the imposition of a ligand field. The ligand field is parameterised using *e* parameters taken from the angular overlap model. These are chemically intuitive: each parameter represents a type of bonding interaction (σ or π bond) and their magnitudes reflect the strength of the metal-ligand interaction [3]. This parameterisation affords real-time calculations, allowing users to explore how changes in the chemical environment affect the spectroscopy. In contrast to DFT's single-determinantal approach, Kestrel's multiconfigurational approach calculates the energies, configurations and spin of all states simultaneously.

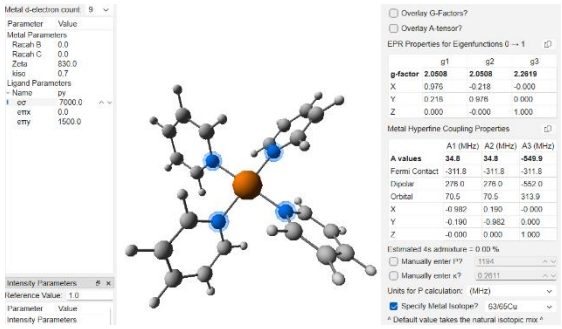

Figure 1. Kestrel's GUI. Parameter values can be varied (left panel) with the spectroscopic results observed in real-time (right panel).

We will demonstrate how Kestrel's chemically meaningful e-values and real-time calculations provide a powerful probe of how changes in the chemical environment of a complex affect its spectroscopy. We will also show how Kestrel can relate EPR parameters to the chemical environment and predict how g and A values are affected by changes in the ligand field.

[1] P. Comba, F. Scherz, G. Nunn, P. H. Walton, *Faraday Discussions* **2022**, *234*, 232-244.

[2] S. Mace, B. S. Grace, M. A. Halcrow, Y. Xu, M. A. Bates, P. H. Walton, B. N. Nguyen, *manuscript in preparation*.

[3] M. Gerloch, Magnetism and ligand-field analysis, Cambridge University Press, Cambridge **1983**.

Poster_22

Spin States in Polymer-Fullerene Organic Solar Cells Explored by Pulse EDMR

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Organic solar cells (OSCs) based on bulk-heterojunction blends of polymer donors and molecular acceptors offer a versatile, low-cost photovoltaic platform with high molecular tunability. Following photoexcitation, excitons diffuse to the donor-acceptor interface, as shown in Figure 1, where charge separation and extraction of free carriers generate electrical power. Despite continued progress, OSC efficiencies remain below the Shockley-Queisser limit, highlighting the need for a molecular-level understanding of performance-limiting loss mechanisms. Electrically Detected Magnetic Resonance (EDMR) spectroscopy addresses this challenge by selectively probing spin-dependent processes directly linked to current generation through resonance-induced changes in device conductivity. By correlating spin excitation with photocurrent, EDMR provides direct insight into spin-dependent charge transport and recombination processes [1].

In this work, spin states governing current generation are investigated in fully assembled polymer-fullerene solar cells at cryogenic temperatures using pulsed EDMR. We considered polymer donors combined with the fullerene acceptor PC61BM for which EPR studies have shown well-separated spectral contributions [2], enabling selective excitation of spins on donor and acceptor molecules. Measurements of EDMR current transients following a π pulse as a function of magnetic field reveal pronounced current quenching across the resonance positions of donor and acceptor, indicating dominant spin-dependent processes that reduce charge carrier population or mobility. Variations in EDMR current transients, spectral line shapes, and nutation behaviour across donor polymers point to distinct underlying spin-dependent mechanisms.

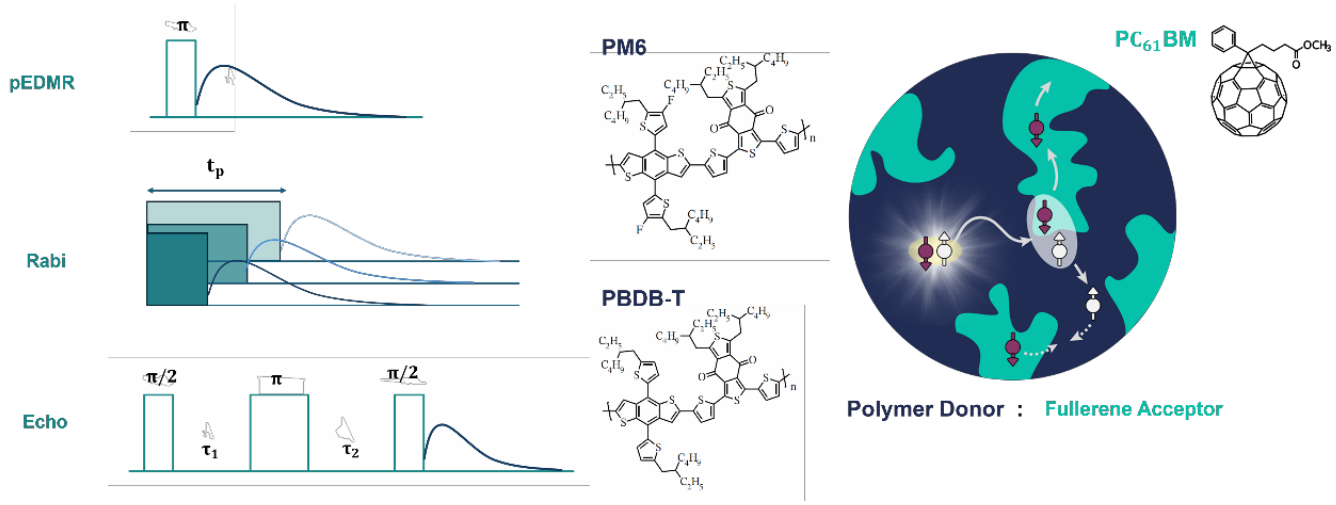

Figure 1. Pulse sequences of the pEDMR, Rabi and EDMR-detected echo experiments with current transient detection used in this work (left). Schematic illustration of the photovoltaic process in the active layer of a bulk heterojunction solar cell (right).

[1] A. Schnegg, *et al.*, *Phys. Chem. Chem. Phys.* **2012**, *14*, 14418–14438.

[2] J. Palmer, *et al.*, *Phys. Chem. Chem. Phys.* **2025**, *27*, 25648-25662.

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