Spin Chemistry Meeting 2026

The 19th International Symposium
On
Spin and Magnetic Field Effects in Chemistry and Related Phenomena

Padova (Italy)
September 20–24, 2026

Book of Abstracts

Welcome to SCM 2026 – Padova

Dear Colleagues,

On behalf of the International Spin Chemistry Committee and the Local Organizing Committee, it is my great pleasure to welcome you to Padova for the 19th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena, known as the "Spin Chemistry Meeting" (SCM).

SCM2026 brings together researchers from around the world to share the latest results in Spin Chemistry, a field built on the surprising fact that electron and nuclear spins can have a profound effect on chemical reactions. As the contributions in this Book of Abstracts show, Spin Chemistry today covers a wide range of themes: from fundamental phenomena like magnetic field effects and hyperpolarization of multi-spin systems, including biological spin chemistry and chirality-induced spin selectivity, to emerging applications in dynamic nuclear polarization using photo-excited states, molecular qubits, novel materials in spintronics, as well as quantum information and sensing. We are especially glad to welcome many students and early-career researchers, whose enthusiasm and new perspectives are essential to the future of this field.

Padova's tradition in spin chemistry goes back to the 1960s, when Giovanni Giacometti founded the first research group in Electron Spin Resonance in Italy. Carried forward by Marina Brustolon and Carlo Corvaja, who chaired the meeting in 2007 on the island of San Servolo in Venice, that tradition continues today in the EPR Group at the Department of Chemical Sciences, working on biological spin chemistry, material science applications, and hyperpolarization.

Beyond the scientific program, Padova invites you to explore its long history, said to begin over 2,500 years ago with Antenor, a legendary hero of the Trojan War. Today, the city is home to the University of Padova, established in 1222, where Galileo Galilei once taught from his wooden lectern at Palazzo Bo. Walking through the city, you can admire Giotto's frescoes in the Scrovegni Chapel, part of Padova's UNESCO-listed Urbs Picta, or take a quiet break under the trees of the Orto Botanico, the world's oldest academic botanical garden.

The social program has been designed with this in mind, taking the conference beyond the lecture halls and into the historic heart of this ancient university city. The exchange of ideas during oral and poster sessions, paired with informal conversations during coffee breaks and social activities, is often where new projects are discussed and fruitful collaborations begin. We hope SCM2026 provides the perfect environment for Spin Chemistry to advance.

Enjoy the conference!

Marilena Di Valentin,

Chair of the Spin Chemistry Meeting 2026

SCM 2026

The 19th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena

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September 20 - 24, 2026

International Spin Chemistry Meeting Committee

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Michael R. Wasielewski (Evanston, USA)
Stefan Weber (Freiburg, Germany)

Spin chemistry Community – https://spin-chemistry-community.github.io/committee/

Local Organizing Committee

Marilena Di Valentin *Conference Chair*
Alessandro Agostini
Antonio Barbon
Marco Bortolus
Donatella Carbonera
Federico De Biasi
Lorenzo Franco
Marco Ruzzi
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Spin Chemistry Meeting 2026 : Timetable

Sunday 20th – Morning

Location: Aula Nievo, Palazzo del Bo, Via VIII Febbraio 1848, 2 Padova

Tutorial Session		
09:45 - 9:50	Opening of Tutorial Session	
9:50 - 11:50	TL 1 Claudia Tait	EPR simulations of spin-polarized systems with EasySpin: From Basics to Advanced Applications

Sunday 20th – Afternoon

Location: Aula Nievo, Palazzo del Bo, Via VIII Febbraio 1848, 2 Padova

12:00 - 17:00	**Guided tours (1 h) of Palazzo del Bo** Several one-hour guided tours of the Palazzo del Bo are offered at hourly intervals
from 14:00	SCM 2026 Registration Desk open

Tutorial Lectures		
14:15 - 15:15	TL2 Christiane Timmel	Product operators, density matrices and friends
15:15 - 16:15	TL3 Michael Wasielewski	Spin chemistry as a probe of chirality-induced spin selectivity (CISS)
16:15 - 17:15	TL4 Nino Wili	Routes to nuclear hyperpolarization

17:45 - 18:00	**Opening of SCM 2026**	
Opening Lecture		
18:00 - 19:00	Ilia Kuprov	Eine neue Kopenhagener Irrlehre: 100 Years of Spin

From 19:30	**Welcome Mixer** at the Restaurant “casa exforo” (Prato della Valle 70a, Padova)

Monday 21st – Morning

Location: Main Lecture Hall (Aula A) – Psico 3 Building; Via Venezia 14, Padova

Session : **Molecular Qubits** *Chair :* ***Yasuhiro Kobori***		
9:00 - 9:40	PL Marco Affronte	Addressing Molecular Spin Qubits by Superconducting Circuits
9:40 - 10:10	IL Alberto Privitera	Light-driven porphyrin-based qubits
10:10 - 10:30	CL Kazunobu Sato	Spin properties of high-spin Mn(II) qubit doped into a metal-organic framework
10:30 - 10:50	CL Stergios Piligkos	Lanthanide coordination complexes for quantum technologies
10:50 - 11:20	**Coffee Break**	
Session : **Electron Spin Polarization** *Chair:* ***Art van der Est***		
11:20 - 11:50	IL Alice Bowen	Adventures in light-induced electron paramagnetic resonance
11:50 - 12:20	IL Claudia Tait	Spin dynamics of charge generation in organic photovoltaic and photocatalytic materials probed by ESR
12:20 - 12:40	CL Gabriel Moise	The spin-polarized photoexcited quartet state of a copper(II) porphyrin
12:40 - 13:00	CL Yuki Kurashige	Photoexcited spin polarization in molecular systems from first principles
Flash Talks *Chair:* ***Marco Bortolus***		
13:05 - 13:10	FT Hanbo Yang	A tale of light and shadow: Room-temperature magnetoluminescence in asymmetric organic biradicals
13:10 - 13:15	FT Joseph Young	Magnetic field effects of radical-exciplex systems
13:15 - 13:20	FT Asato Mizuno	Elucidation of spin-correlated emission of a carbazole-containing diradical emitter
13:20 - 13:25	FT Ziqiu Huang	Host-guest Crystal Engineering Tailors the Room Temperature Spin Dynamics in Molecular Quantum Materials
13:30 – 15:00	**Lunch**	

Monday 21st Afternoon

Location: Main Lecture Hall (Aula A) – Psico 3 Building; Via Venezia 14, Padova

Session: **Dynamic Nuclear Polarization** *Chair:* ***Silvia Cavagnero***		
15:00 - 15:30	IL Gabriele Stevanato	Enhanced ^{1}H and ^{19}F NMR microwave-free optical hyperpolarization in liquids
15:30 - 15:50	CL Moreno Lelli	Accurate large spin ensemble simulations of high-field and fast-MAS solid-state dynamic nuclear polarization NMR
15:50 - 16:10	CL Claudia Avalos	Optically excited molecules for DNP applications
Flash Talks *Chair:* ***Alfonso Zoleo***		
16:15 - 16:20	Thowfik Salam	Perylene Diimide(PDI) Based Chromophore-Radical Architectures for Long-Lived Photoexcited Spin States and as Promising Molecular Qubit Candidates
16:20 - 16:25	Margrete Henrichsen	Simple 3d-metal complexes for Magnetic Refrigeration
16:25 - 16:30	Meenu Solly	Electrically Detected Magnetic Resonance Characterisation of Donors in Silicon
16:30 - 16:35	Lorenzo Catini	Using spin as a probe to understand charge recombination in organic solar cells: an EDMR study
16:35 - 16:40	Trent McHenry	Triplet Pathways in Twisted Crystalline Diketopyrrolepyrrole Films
16:40 - 16:45	Angelo Carella	Photoinduced spin interactions and dynamics in a copper(II)-free base porphyrin dimer
16:45 - 16:50	Damyan Frantzov	Room-temperature molecular quantum sensing of the Earth's magnetic field
16:50 - 16:55	Paul Mentzel	Organic Carbenes as a Single Molecule Spin-Photon Interface
16:55 - 17:00	Wataru Ishii	Modular spin-optical interface in persistent molecular spin qubits
17:00 - 17:05	Matteo Lanza	Quantum sensing of time-dependent magnetic signals with molecular spins
17:05 - 17:10	Oliver Christie	Magneto-Optical Effects in Organic Radicals
17:10 - 17:15	Taichi Hiramoto	Circularly polarized luminescence from a polybrominated triarylmethyl radical with a pyridyl ring

Session: **Charge and Spin in Molecular Materials** *Chair:* ***Antonio Barbon***		
17:20 - 17:40	CL Mercè Deumal	Towards the conductivity-magnetism interplay in hydroxylated ethylene-coupled tetrathiofulvalenes and nitronyl nitroxides for magnetoresistance application
17:40 - 18:00	CL Raanan Carmieli	EPR study of charge transfer co-crystals structure/function relationship
18:00 - 20:00	**Poster Session 1 (Odd Poster nr.)** & **Networking Reception**	

Tuesday 22nd – Morning

Location: Main Lecture Hall (Aula A) – Psico 3 Building; Via Venezia 14, Padova

Session : **Photo-CIDNP** *Chair :* ***Stefan Weber***		
9:00 - 9:40	PL Lyndon Emsley	Nuclear hyperpolarization in synthetic donor–acceptor dyes by photo-chemically induced dynamic nuclear polarization
9:40 - 10:10	IL Jörg Matysik	Studying the solid-state photo-CIDNP effect
10:10 - 10:40	IL Silvia Cavagnero	LC-photo-CIDNP: a gateway to hypersensitive NMR spectroscopy
10:40 - 11:00	CL Ilia Kuprov	Chemical hydrodynamics of nuclear spin states
11:00 - 11:30	**Coffee Break**	
Session : **Quantum Information and Sensing** *Chair:* ***Dane McCamey***		
11:30 - 12:00	IL Malcolm Forbes	Two's company, three's not a crowd: creation and control of multi-spin systems for quantum information science applications
12:00 - 12:20	CL Sarah Mann	From electron to nuclear spins: Room-temperature optically detected coherent control in chemically tunable molecular qubits
12:20 - 12:40	CL Qi Zhang	Single-molecule-scale magnetic resonance with solid spin quantum sensors
12:40 - 13:00	CL Naitik Panjwani	Engineering nuclear spin environments for molecular spin coherence: a multifrequency EPR study on luminescent perhalofluoro trityl radicals
Flash Talks *Chair:* ***Alessandro Agostini***		
13:05 - 13:10	FT Máté Visegrádi	Enhancements of Over a Factor 1000 by Rational Design of photo-Polarization Agents for Dye Sensitized Solid-state NMR
13:10 - 13:15	FT Toshiteru Tada	Efficient Electron Transfer Employs High-Performance in photo-CIDNP
13:15 - 13:20	FT Federico De Biasi	Optical hyperpolarization of ^{1}H and ^{19}F spins in organic liquids
13:20 - 13:25	FT Marco Tommaso Barreca	Organic Diradicals Bridged by Inverted Singlet - Triplet Units for Optical - Spin Interfaces
13:30 – 14:45	**Lunch**	

Tuesday 22nd - Afternoon

Location: Main Lecture Hall (Aula A) – Psico 3 Building; Via Venezia 14, Padova

Session: **Radical Spin Chemistry** *Chair:* ***Jörg Matysik***		
14:45 – 15:00	SL Optoprim - Magnitude Instruments	Pushing the Boundaries in Transient Absorption Spectroscopy
15:00 - 15:20	CL Hadi Zadeh-Haghighi	Magnetic field dependent isotope effect in tubulin polymerization
15:20 – 15:40	CL Li-Nan Zhou	Spin regulation strategies for enhancing photoredox catalysis
Flash Talks *Chair:* ***Gabriele Stevanato***		
15:45 - 15:50	Marco Flores	Is there direct electron transfer from A_0 to F_X in the reaction center from *Heliobacterium modesticaldum*?
15:50- 15:55	Pedro Alvarez	Limits on the precision of radical pair magnetoreception in the avian retina
15:55- 16:00	Boris Gribakin	Ultrafast vibrational spectroscopy of migratory songbird cryptochrome
16:00 - 16:05	Nicole Höfer	Separation of spin species based on echo shape for pulsed EPR
16:05 - 16:10	Mikhail Kolokolov	Laser-induced dipolar EPR combined with molecular modeling for structural studies of protein-ligand complexes
16:10 - 16:15	Christopher Einholz	Optimization of Magnetic Field Effects - from Magnetoreception to Biological Spin Qubits
16:15 - 16:20	Ruonan Qin	Light-induced ^{1}H hyperpolarization produced by flavoprotein at 4.7 Tesla
16:20 - 16:25	Andrea Calcinoni	Probing electron transfer directionality in Far-Red PSI reaction centre by EPR spectroscopy
16:25 - 16:30	Giulia Da Ros	Genetic encoding of non-canonical amino acids in electron transport protein complexes: moving towards protein structural determination in cellular environments using EPR
16:30 - 16:35	Amina Mouhamed	Lithium isotope effects and magnetic interactions in flavin-ascorbyl radical pairs
16:35 - 16:40	Takema Hikawa	Energy-transfer-modulated Magnetoluminescence for a five-coordinated Mn^{II} complex in organic host matrices
16:40 - 16:45	Xinyi Shen	Symmetry-Breaking Modulation of Platinum Sites in Multicomponent Alloy for Efficient Oxygen Reduction Reaction

Session: **Biological Spin Chemistry** *Chair:* ***Donatella Carbonera***		
16:50 - 17:20	IL Stefan Weber	Electron and nuclear hyperpolarization in blue-light activated proteins: a radical pair perspective
17:20 - 17:40	CL Gerd Kothe	Nanosecond structure of radical pair intermediates from high-frequency quantum oscillations. Elucidation of the $Q_A^{\bullet-}$ to Q_B electron transfer step in purple bacterial photosynthesis
17:40 - 17:55	SL Cinquepascal	Cooling the Spin: Cryogenic Platforms for EPR, Parahydrogen Production and Quantum Science
18:00 - 20:00	**Poster Session 2 (Even Poster nr.)** & **Networking Reception**	

Wednesday 23rd - Morning

Location: Main Lecture Hall (Aula A) – Psico 3 Building; Via Venezia 14, Padova

Session : **Qubits & Quantum Sensing** *Chair :* ***Malcom Forbes***		
9:00 - 9:40	PL Nobuhiro Yanai	From molecular qubits to quantum sensors through materials chemistry
9:40 - 10:10	IL Dane McCamey	Spatially resolved coherence of organic molecular spins at room temperature
Session : **Magnetic-Field Effects** *Chair :* ***Malcom Forbes***		
10:10 - 10:30	CL Christopher Lambert	Magnetic-field-dependent delayed fluorescence form thermally activated reverse charge separation of spin-correlated charge separated states
10:30 - 10:50	CL Ryota Matsuoka	Spin-state-dependent photophysics of a spatially confined luminescent diradical and its magnetic modulation
10:50 - 11:20	**Coffee Break**	
Session : **CISS Effect** *Chair:* ***Michael Wasielewski***		
11:20 - 11:50	IL Stefano Carretta	Molecular spins and chirality as resources for quantum technologies
11:50 - 12:20	IL Yasuhiro Kobori	Chirality-induced spin selectivity in photoinduced charge separations of cryptochrome for magnetoreception
Session : **Novel Techniques in Biological Spin Chemistry** *Chair:* ***Michael Wasielewski***		
12:20 - 12:50	IL Stuart Mackenzie	New approaches for studying magnetic field effects in radical pair chemistry
12:50 - 13:20	IL Jonathan Woodward	Magnetic field effect microscopy on radical pairs in biological systems
13:25 – 14:50	**Lunch**	

Wednesday 23rd Afternoon

15:00	**Excursion and social events**

Thursday 24th - Morning

Location: Main Lecture Hall (Aula A) – Psico 3 Building; Via Venezia 14, Padova

Session : **Qubits & Quantum Sensing** *Chair :* ***Dane McCamey***		
9:00 - 9:40	PL Arzhang Ardavan	Engineering molecular-spin-based quantum technologies
9:40 - 10:10	IL Peter Maurer	From diamond defects to protein-based qubit sensors
Session : **Spin-coupled Systems** *Chair :* ***Dane McCamey***		
10:10 - 10:30	CL Susanna Ciuti	Light-induced behavior of Cr-based antiferromagnetically-coupled heterometallic systems
10:30 - 10:50	CL Jordi Ribas	Electric-field control of spin-exchange couplings in organic diradicals and 2D covalent organic frameworks
10:50 - 11:20	**Coffee Break**	
Session : **Chromophore–Radical Systems** *Chair:* ***Kiminori Maeda***		
11:20 - 11:50	IL Michael Wasielewski	Triplet diradical optical-spin interfaces for quantum sensing
11:50 - 12:20	IL Art van der Est	Using spin polarization and transient EPR to study charge separation in Al(III) porphyrin homodimer–fullerene supramolecular assemblies
12:20 - 12:40	CL Yuri Kandrashkin	Systematics of photoinduced spin dynamics in rigid chromophore–radical compounds
12:40 - 13:00	CL Kieran Richards	Designing radicals for upconversion: Substitution effects of rylene chromophores
13:00 - 13:20	CL Danillo Valverde	Toward blue emission in radical emitters: TEMPO radical coupled to TADF and INVEST scaffolds
13:25 – 14:45	**Lunch**	

Thursday 24th - Afternoon

Location: Main Lecture Hall (Aula A) – Psico 3 Building; Via Venezia 14, Padova

Session: **Magnetic Field Effects** *Chair:* ***Christiane Timmel***		
14:45 - 15:15	IL Kiminori Maeda	Coherent spin dynamics and low field effect
15:15 - 15:45	IL Tomoaki Miura	Magnetically enhanced photocurrent in organic photovoltaic materials due to spin-polarized triplet states
15:45 - 16:05	CL Hohjai Lee	Spin-selective photochemistry: magnetic control of singlet oxygen through upstream radical-pair dynamics
Session: **Biological Spin Chemistry** *Chair:* ***Christiane Timmel***		
16:05 - 16:25	CL Dominik Bucher	Optically detected and radio wave-controlled spin chemistry in flavoproteins
16:25 - 16:45	CL Erik Schleicher	Modifying the photochemistry of flavoproteins
16:45 – 17:15	**Coffee Break**	
Session: **Triplets & High-Spin States** *Chair:* ***Lorenzo Franco***		
17:15 - 17:45	IL Jenny Clark	Singlet exciton fission and triplet-triplet annihilation studied with transient magneto-optical spectroscopy
17:45 - 18:15	IL Jeannine Grüne	Optical readout of molecular high-spin states at room temperature
18:15 - 18:35	CL Alejandro de Sousa	Room temperature optical read-out of triplet states in (6,5) SWCNTs
18:35 - 18:50	**Closing Remarks and annoucement of SCM 2028**	
20:30	**Social Dinner** at the Restaurant “Isola di Caprera” (Via Marsilio da Padova 11, Padova)	

PL - Plenary Lecture: 35 + 5 minutes

IL - Invited Lecture: 25 + 5 minutes

CL - Contributed Lecture: 15 + 5 minutes

Flash talks - 5 minutes (3 slides max)

List of Posters

Poster + Flash Talk
Poster Only

1	**Abdullin** Dinar	**Ulm** Germany	Toward Enhanced Photoluminescence in Luminescent Organic Diradicals
2	**Agostini** Alessandro	**Padova** Italy	ODMR reveals enhanced Carotenoid–Chlorophyll coupling and triplet quenching in Siphonous green algal Light-Harvesting Complexes
3	**Alvarez** Pedro	**Oldenburg** Germany	Limits on the precision of radical pair magnetoreception in the avian retina
4	**Ando** Rempei	**Abu Dhabi** United Arab Emirates	Investigating the Effects of Deuteration and Host Matrix on the Spin Dynamics of Photogenerated PDI-BDPA
5	**Anisimova** Irina	**Oldenburg** Germany	Unifying Spin Dynamics for Magnetic Resonance: High-Performance Simulations and Analysis via Web-Based Toolkit
6	**Barreca** Marco Tommaso	**Parma** Italy	Organic Diradicals Bridged by Inverted Singlet – Triplet Units for Optical – Spin Interfaces
7	**Bruyers** Dominic	**Freiburg** Germany	Influence of the radical properties in triplet–radical spin-polarization transfer
8	**Calcinoni** Andrea	**Padova** Italy	Probing electron transfer directionality in Far-Red PSI reaction centre by EPR spectroscopy
9	**Carella** Angelo	**Firenze** Italy	Photoinduced spin interactions and dynamics in a copper(II)-free base porphyrin dimer
10	**Carlotti** Benedetta	**Perugia** Italy	Singlet Fission in H/J Diketopyrrolopyrrole Aggregates under the Gaze of Time Resolved Optical and Magnetic Spectroscopy
11	**Catini** Lorenzo	**Oxford** UK	Using spin as a probe to understand charge recombination in organic solar cells: an EDMR study
12	**Christie** Oliver	**Swansea** UK	Magneto-Optical Effects in Organic Radicals
13	**Clark** Jonathon	**Oxford** UK	Spin Polarisation of Gadolinium Complexes by Photoexcited Rhenium Chromophores
14	**Colegate** Benjamin	**Manchester** UK	Molecular Alignment in Liquid Crystals for Improving Gate Fidelity in Molecular Electron Spin Qubits
15	**Cubbin** Daniel	**Oxford** UK	Avian Cryptochrome Photochemistry: Sensing vs Signalling

16	**Da Ros** Giulia	**Manchester** UK	Genetic encoding of non-canonical amino acids in electron transport protein complexes: moving towards protein structural determination in cellular environments using EPR
17	**De Biasi** Federico	**Padova** Italy	Optical hyperpolarization of 1H and 19F spins in organic liquids
18	**Denisov** Dmitry	**Leipzig** Germany	Investigating Secondary Polarization Transfer in Flv-Pro$_n$-Trp Diads by Liquid-State ^{1}H Photo-CIDNP NMR
19	**Eckvahl** Hannah	**Oxford** UK	Bimetallic Lanthanide Complexes as Tuneable Molecular Spin Qubit Candidates
20	**Einholz** Christopher	**Munich** Germany	Optimization of Magnetic Field Effects – from Magnetoreception to Biological Spin Qubits
21	**Fabris** Luca	**Padova** Italy	BisNHC-Rhodium Complexes for Parahydrogen Induced Polarization
22	**Famulari** Antonino	**Oxford** UK	Unravelling the Photocatalytic Mechanism of a BODIPY–Rhenium CO_2 Reduction Photocatalyst by EPR Spectroscopy
23	**Faramawy** Ahmed	**Padova** Italy	Towards Fully Automated Benchtop NMR: An Integrated System for Hyperpolarization and Optical Polarization
24	**Felice** Assunta	**Oxford** UK	Investigation of Spin Dependent Processes in Polymer-Fullerene Organic Solar Cells by Pulsed EDMR.
25	**Fella** Fabian	**Würzburg** Germany	Magnetic High Field Effects in Chalcogen Substituted NDI Donor-Acceptor Dyads
26	**Floreani** Federico	**Padova** Italy	Efficient ^{15}N SABRE Hyperpolarization of Nicotine Derivatives in Fluorocarbon
27	**Flores** Marco	**Tempe** USA	Is there direct electron transfer from A_0 to F_X in the reaction center from *Heliobacterium modesticaldum*?
28	**Frantzov** Damyan	**Oxford** UK	Room-temperature molecular quantum sensing of the Earth's magnetic field
29	**Galuppo** Giovanna	**Manchester** UK	Toward Optical Control of Molecular Spin Qubits: Time-Resolved EPR of Porphyrin-{Cr_7Ni} Assemblies
30	**Gribakin** Boris	**Oldenburg** Germany	Ultrafast vibrational spectroscopy of migratory songbird cryptochrome
31	**Groß** Tobias	**Würzburg** Germany	From π-conjugated to σ-aromatic and aliphatic bridges: Modulating electron transfer and spin chemistry in donor-bridge-acceptor dyads

32	**Gwynn** Tristen	**Stellenbosch** South Africa	Conditional Enhancement of Radical Pair Dynamics via Chiral State Preparation
33	**Hayashi** Natsuki	**Osaka** Japan	Spin Relaxation in Pyridyl-Containing Luminescent Triarylmethyl Radicals
34	**Henrichsen** Margrete	**Copenhagen** Denmark	Simple 3d-metal complexes for Magnetic Refrigeration
35	**Hikawa** Takema	**Osaka** Japan	Energy-transfer-modulated Magnetoluminescence for a five-coordinated Mn^{II} complex in organic host matrices
36	**Hiramoto** Taichi	**Osaka** Japan	Circularly polarized luminescence from a polybrominated triarylmethyl radical with a pyridyl ring
37	**Höfer** Nicole	**Berlin** Germany	Separation of spin species based on echo shape for pulsed EPR
38	**Huang** Ziqiu	**London** UK	Host-guest Crystal Engineering Tailors the Room Temperature Spin Dynamics in Molecular Quantum Materials
39	**Imran** Muhammad	**Halle** Germany	A Concealed Non-Kekulé Nanographene as an Addressable Molecular Spin Qubit
40	**Ishii** Wataru	**Tokyo** Japan	Modular spin-optical interface in persistent molecular spin qubits
41	**Ito** Takuma	**Kyoto** Japan	Theoretical Calculation of Fermi's Golden Rule Rate Including the Anharmonicity of Potential Energy Surfaces
42	**Ki** Yeongcheol	**Gwangju** Republic of Korea	Upstream Spin-Dependent Modulation of Singlet Oxygen Generation through Radical Pair Dynamics
43	**Kolokolov** Mikhail	**Novosibirsk** Russia	Laser-induced dipolar EPR combined with molecular modeling for structural studies of protein-ligand complexes
44	**Kuhn** Lars	**Freiburg** Germany	Hyperpolarisation-Enhanced NMR Spectroscopy of Unaltered Biofluids Using photo-CIDNP
45	**Ladwig** Marco	**Freiburg** Germany	Time-resolved EPR spectroscopy of modified cryptochromes
46	**Lanza** Matteo	**Modena** Italy	Quantum sensing of time-dependent magnetic signals with molecular spins
47	**Lazzarin** Francesco	**Padova** Italy	Rationalization of electron spin polarization transfer in chiral porphyrin-[6]helicene-TEMPO triads
48	**Leggatt** Sam	**Oxford** UK	Exploring Porphyrin Triads as Molecular Compasses

49	**Mamusi** Fatemeh	**Barcelona** Spain	Insights into the structure–property relationships governing magnetoluminescence in Non-Kekulé triarylmethyl diradicals
50	**Matsushita** Yoshitoshi	**Saitama** Japan	Selective Observation of Radical Pair Spin Dynamics Using Pump–Push Spectroscopy
51	**McHenry** Trent	**New York** USA	Triplet Pathways in Twisted Crystalline Diketopyrrolepyrrole Films
52	**Mentzel** Paul	**Ulm** Germany	Organic Carbenes as a Single Molecule Spin-Photon Interface
53	**Miyokawa** Katsuki	**Kyoto** Japan	Predicting Electron Spin Relaxation Rates of Triplet Chromophores from Molecular Dynamics
54	**Mizuno** Asato	**Osaka** Japan	Elucidation of spin-correlated emission of a carbazole-containing diradical emitter
55	**Mouhamed** Amina	**Guildford** UK	Lithium isotope effects and magnetic interactions in flavin-ascorbyl radical pairs
56	**Munguía Salazar** Paloma	**Devon** UK	The Semiquinone as a Distinct Structural State in the *Erithacus rubecula* Cryptochrome 4a Photocycle
57	**Murton** Patrick	**Edinburgh** UK	Exploring the Sensitivity Limits of Nanodiamond Quantum Sensors for Biomedical Applications
58	**Musabirova** Guzel	**Leipzig** Germany	Magnetic-Field Effects in Photo-CIDNP of Flavin-Tryptophan Dyads
59	**Nakagawa** Sakura	**Swansea** UK	Open-Shell Carbene-Metal-Amide Emitter for Intramolecular Triplet–Doublet Interactions
60	**Olavesen** Carl	**Oxford** UK	The effect of isotopic substitution on magnetic field effects in avian cryptochromes
61	**Ono** Shogo	**Tokyo** Japan	Mechanistic analysis of MagLOV toward its application as a protein-based quantum sensor
62	**Pearse** Cass	**Exeter** UK	Revisiting Electron-Electron Dipolar Interactions in Geminate Radical Pairs: An Approach Based on the Stochastic Liouville Equation
63	**Piccolo** Anna	**Padova** Italy	CW-EPR applied to Heritage Science: insights into the degradation mechanism of celluloid
64	**Qin** Ruonan	**Leipzig** Germany	Light-induced 1H hyperpolarization produced by flavoprotein at 4.7 Tesla
65	**Redman** Ashley	**Ulm** Germany	Spin communication in TTM-based chromophore—radical systems

66	**Salam** Thowfik	**Abu Dhab** United Arab Emirates	Perylene Diimide(PDI) Based Chromophore-Radical Architectures for Long-Lived Photoexcited Spin States and as Promising Molecular Qubit Candidates
67	**Selby** Dan	**Manchester** UK	Optical Dynamic Nuclear Polarisation in Solution-state Magnetic Resonance
68	**Shen** Xinyi	**Hefei** China	Symmetry-Breaking Modulation of Platinum Sites in Multicomponent Alloy for Efficient Oxygen Reduction Reaction
69	**Soga** Shogo	**Saitama** Japan	EPR study of mononuclear iron centers in ISCA1 related to magnetic field response
70	**Solly** Meenu	**Manchester** UK	Electrically Detected Magnetic Resonance Characterisation of Donors in Silicon
71	**Sowa** Ryosuke	**Kyoto** Japan	Small Singlet-Triplet Gaps: A Multireference Electronic Structure Study using Trimethylenemethane-Type Biradicals as Model Systems
72	**Tada** Toshiteru	**Fukuoka** Japan	Efficient Electron Transfer Employs High-Performance in photo-CIDNP
73	**Tesiman** Calysta	**London** UK	Bridge conjugation towards control of spin multiplicity in mesitylated trityl biradicals
74	**Toninato** Jacopo	**Padova** Italy	EPR Characterization of Peroxy Radicals in Industrially Irradiated PTFE
75	**Visegrádi** Máté	**Lausanne** Switzerland	Enhancements of Over a Factor 1000 by Rational Design of photo-Polarization Agents for Dye Sensitized Solid-state NMR
76	**Wiech** Mathias	**Graz** Austria	Toward a Quantitative Assessment of Photoreactions by NMR
77	**Yang** Hambo	**Swansea** UK	A tale of light and shadow: Room-temperature magnetoluminescence in asymmetric organic biradicals
78	**Young** Joseph	**Swansea** UK	Magnetic field effects of radical-exciplex systems
79	**Yun** Ena	**Evanston** USA	Optical Spin Polarization via Spin-Selective Charge Recombination in Luminescent Non-covalent TTM Diradicals
80	**Zambon** Roberto	**Padova** Italy	Theoretical Insights into Non-Equilibrium Spin Polarization in Triplet States through Lindblad dynamics
81	**Zhou** Zhaobo	**Prague** Czech Public	Ultrafast light control of magnetization dynamics in altermagnets

Talks

Opening Lecture

"Eine neue Kopenhagener Irrlehre": 100 Years of Spin

Ilya Kuprov

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School of Chemistry and Chemical Engineering, University of Southampton, UK.

We do not know if Pauli had ever apologised to Ralph Kronig for talking him out of proposing spin in 1925 – the same idea had been published only a few months later (to universal puzzlement) by Uhlenbeck and Goudsmit who had lost a factor of two that had taken another year to find... We never tell these stories at spin chemistry conferences! Well, now that it's been exactly 100 years, I have an excuse. Here comes a history lesson.

(1922): Two spots and a mild panic
Stern-Gerlach experiment – an observational coup immediately celebrated as a proof that, well... something is quantised. Nobody knows exactly what.

(1924 – Early 1925): Pauli states the obvious
Pauli proclaims that electrons possess a mysterious "two-valued degree of freedom", inventing the exclusion principle and the phrase "classically indescribable."

(Jan 1925): Kronig's cautionary tale
Ralph Kronig proposes to Pauli that electrons might actually spin. A quick calculation reveals a factor-of-two discrepancy in the predicted fine structure of the hydrogen spectrum. Pauli rubbishes the proposal; Kronig abandons the idea.

(Nov 1925): Two students and a hydrogen spectrum
George Uhlenbeck and Samuel Goudsmit – both graduate students, and thus immune to prudence – publish a note proposing electron spin (Ehrenfest, their supervisor, had posted the manuscript to a journal before they could reconsider). Lorentz sends a courteous list of devastating classical objections, Pauli rolls his eyes, Bohr mutters something non-committal... the missing factor of 2 roams the corridors.

(Apr 1926): Relativity to the rescue
Llewellyn Thomas revisits the arithmetic and realises that a relativistic kinematic wobble – later called Thomas precession – halves the effective spin-orbit coupling. The numbers now match experiment. Pauli performs a dignified U-turn, produces the eponymous matrices, and insists that had always been the plan.

(1928 –1932): Dirac and Wigner pull the curtains
Paul Dirac guesses an equation out of which spin falls out automatically, $g = 2$ emerges without effort, and antimatter appears as a side effect. Eugene Wigner derives the equation from basic symmetries of physical reality.

This is more of a historical / educational lecture than a scientific one. An important point that we will cover though is what *exactly* spin is – cutting through the rampant confusion that reigns in the textbooks and on the internet.

Plenary Lecture

Addressing Molecular Spin Qubits by Superconducting Circuits

M. Affronte[1,2], C. Bonizzoni[1,2], M. Lanza[1,2], A. Ghirri[2]

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[2] *Istituto Nanoscienze—CNR, Centro S3, via G. Campi 213/A, Modena 41125, Italy*

Coherent manipulation of electron and nuclear spins in molecular systems is the prerequisite for applications such as quantum computing [1] or sensing [2]. One route to achieve this goal is to embed molecular spins in superconducting circuits exploiting the complementary advantages offered by each system in a scalable architectures. To this end, we developed a multifrequency platform based on high-Tc YBCO superconducting planar resonators [3] and home-made heterodyne systems for non-conventional multifrequency spectroscopy [4, 5]. This platform allows us to tackle current challenges for the use of molecular spin for quantum technologies.

I shall first address the problem of quantum sensing. For this, we developed and tested protocols for measuring tiny external magnetic fields with solely microwave pulses and detecting the phase accumulation in echo signal. This method allows us to get magnetic field sensitivity as high as $nT/\sqrt{Hz}$ [6]. We have extended these protocols to reconstruct tiny magnetic field signals with different time evolution with similar sensitivity that is what we need to measure a flip-flop process in a nearby analyte [7].

Secondly, we implement our setup to separately address electron and nuclear spins in molecular qubits by sequences of alternating RF and MW pulses. To test this, we performed Electron Nuclear DOuble Resonance (ENDOR) experiments and show the readout of the ^{51}V nuclear spin transitions through the electronic spin echo. Further experiments with a dedicated RF-MW pulse sequence demonstrated that electronic phase coherence can be stored in the nuclear spins and retrieved (Storage and Retrieval) after a total free precession time that greatly exceeds the electronic phase memory time [8]. This result establishes a new route for encoding quantum information on both electronic and nuclear degrees of freedom of a chemically tuneable platform.

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Invited Lecture

Light-driven porphyrin-based qubits

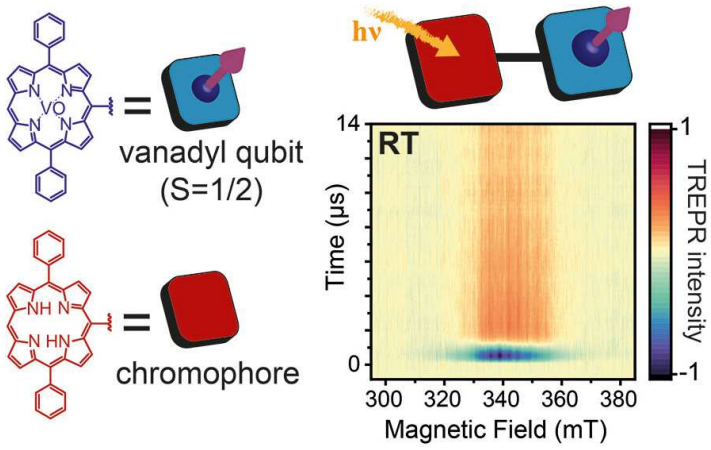
Alberto Privitera[1]

[1]*Department of Industrial Engineering, University of Florence, Italy*

Molecular qubits based on porphyrins offer a modular platform for quantum information science due to their excellent coherence properties, multiple nuclear spin levels, and their surface-processability.[1] However, important challenges remain, including spin initialization at temperatures above the sub-kelvin regime and the realization of scalable architectures through the controlled, ultrafast activation of interqubit interactions.

Here, I will present how light-driven interactions can contribute to addressing these open challenges.[2-3] By tailoring the chemistry of porphyrin-based systems, photoexcitation of free-base porphyrin chromophores coupled to vanadyl porphyrin qubits ($V^{IV}O$, S=½) can generate multispin states with spin polarization that persists up to room temperature. The combination of transient absorption spectroscopy, time-resolved electron paramagnetic resonance (TREPR), density functional theory (DFT), and theoretical modelling provides insight into the light-driven spin dynamics and reveals the potential of photoinduced processes for spin initialization and controlled spin coupling in molecular qubit systems.

This work is supported by the European Research Council (ERC Starting Grant LIGHT-QIS, Project No. 101219747).



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Contributed Lecture

Spin Properties of High-Spin Mn(II) Qubit Doped into a Metal-Organic Framework

Kazunobu Sato[1], Takeshi Yamane[1], Shraddha Gupta[2], Masanori Wakizaka[3], and Masahiro Yamashita[4,5]

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Molecule-based spin qubits are emerging as new candidates for quantum-information processing (QIP). They exhibit great promise as quantum bits (qubits) due to their well discrete quantum properties. Furthermore, their high chemical tunability and easy surface deposition properties suggest several potential advantages to be incorporated for QIPs, over the more extensively explored solid-state qubits such as diamond nitrogen vacancy centers and SiC divacancies. Scalability due to self-organization includes the ability for the interactions among molecular qubits to be systematically manipulated at the synthetic level through controlled processes. And the capacity of the individual qubit monomers to be assembled into extensive, well-organized arrays, such as two-dimensional (2D) and three-dimensional (3D) lattices, is a great attraction.

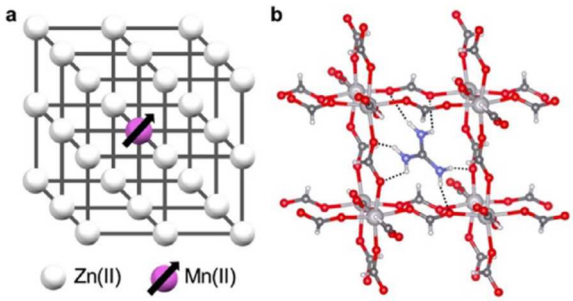

Fig.1 (a) Conceptual illustration of the Mn(II)-doped Zn(II)-based MOF.
(b) Crystal structure of the host Zn(II)-MOF.

In this paper, we present spin properties and dynamics of Mn(II) ion qubit doped in the diamagnetic Zn-MOF, discussing the spin relaxation times as studied by pulsed EPR spectroscopy as well as electron-spin transient nutation spectroscopy[1]. Figure 2 shows temperature dependence of spin relaxation times T_1 and T_2 determined for the Kramers transitions of the 0.02% Mn(II)-doped Zn(II)-MOF. We will also discuss the field dependent relaxation times of the Mn(II) qubit, comparing the spin relaxation of other qubit systems based on MOF[2,3].

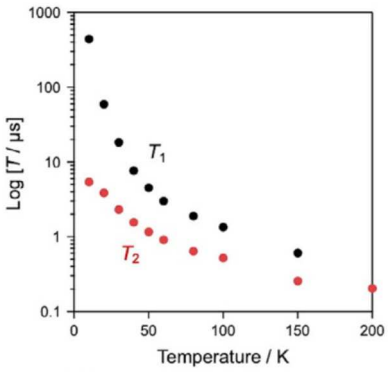

Fig.2 Relaxation times T_1 and T_2 of Mn(II)-doped Zn(II)-MOF

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Contributed Lecture

Lanthanide Coordination Complexes for Quantum Technologies

Stergios Piligkos[1]

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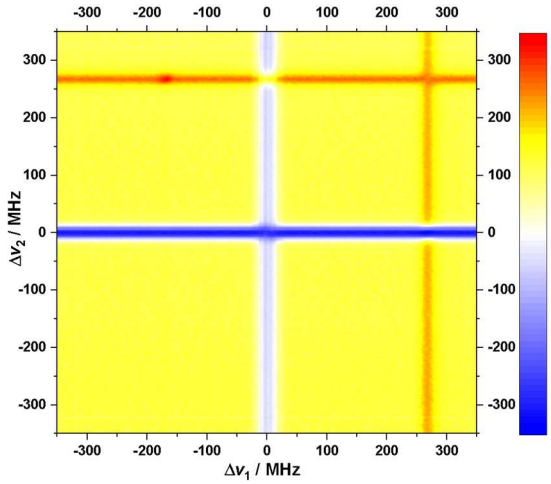
In recent years we have shown, that Lanthanide-based coordination complexes hold potential for use as physical supports for the implementation of single- and entangled-qubit quantum gates within the context of Quantum Information Technology.[1-8]
A crucial advantage of molecular magnetic materials with respect to other quantum hardware platforms is that they often behave as electronic or electronuclear Qudits, that is they often possess more than two low-lying addressable quantum states which offers the possibility to efficiently implement two-qubit gates,[9] quantum error correction algorithms,[2] quantum simulators[5] and quantum algorithms.[8]

We present herein variable microwave multi-frequency pulse sequences that aim to establish an all-to-all connectivity in purely electronic molecular Qudit spaces, exemplified by the S = 7/2 ground state of Gd(III) in Gd(trensal).

We thank the Novo Nordisk Foundation for research grants NNF20OC0065610 and NNF21OC0068806.



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Invited Lecture

Adventures in Light-induced Electron Paramagnetic Resonance

Susanna Ciuti[1], Giulia Da Ros[1], Giovanna Galuppo[1], Andrew Sugden[1], Lubomir Loci[1], Selena J. Lockyer[1], Arianna Cantarella[2,3], D.K. Andrea Phan Huu[2], Alessandro Chiesa[2,3,4], Grigore A. Timco[1], Olivia Churchill[1], Oleksandr Kanibolotskyy[5], Mor Tsfania[1], George F. S. Whitehead[1], Derren Heyes[6], Adam Brookfield[1], Arnau Bertran[1], Jack Sawyer[1], Ciarán J. Rogers[1], Fabio Santanni[7], Roberta Sessoli[7], Alberta Ferrarini[8], Marta De Zotti[8], Pete Skabara[5], Alexander Golovanov[1], Sam Hay[6], Anthony Green[6], Eric J. L. McInnes[1], Stefano Carretta[2,3,4], Richard E. P. Winpenny[1], Marilena Di Valentin[8], Alice M. Bowen[1]

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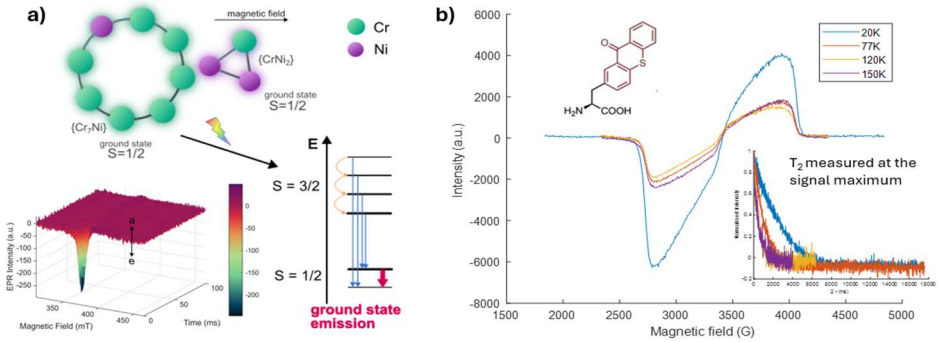
Light-induced Electron Paramagnetic Resonance (EPR) has significant potential applications from quantum information processing (QIP) to distance measurements in biological systems that might lead to new in-cell methodologies [1]. We explore how antiferromagnetic coupling in multi-metallic transition metal clusters with spin-½ (S = ½) ground states can lead to polarization of these states upon optical excitation (figure a) [2]. These have potential applications as switches in QIP and interestingly have polarization that lives longer than the T_1 in the dark ground state. Secondly, we present results using chromophores and non-canonical amino acids, which form triplet states upon optical excitation, with measurable Hahn echoes and T_2 lifetimes that are favourable for Light-induced Pulsed Dipolar Spectroscopy (LiPDS, figure b).



a) *Optical excitation of Cr(III)-Ni(II) coupled cluster systems leads to long-lived polarisation of the ground state doublet.*

b) *Thioxanthone based non-cannonical amino acids have long lived triplet states with properties suitable for LiPDS.*

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Invited Lecture

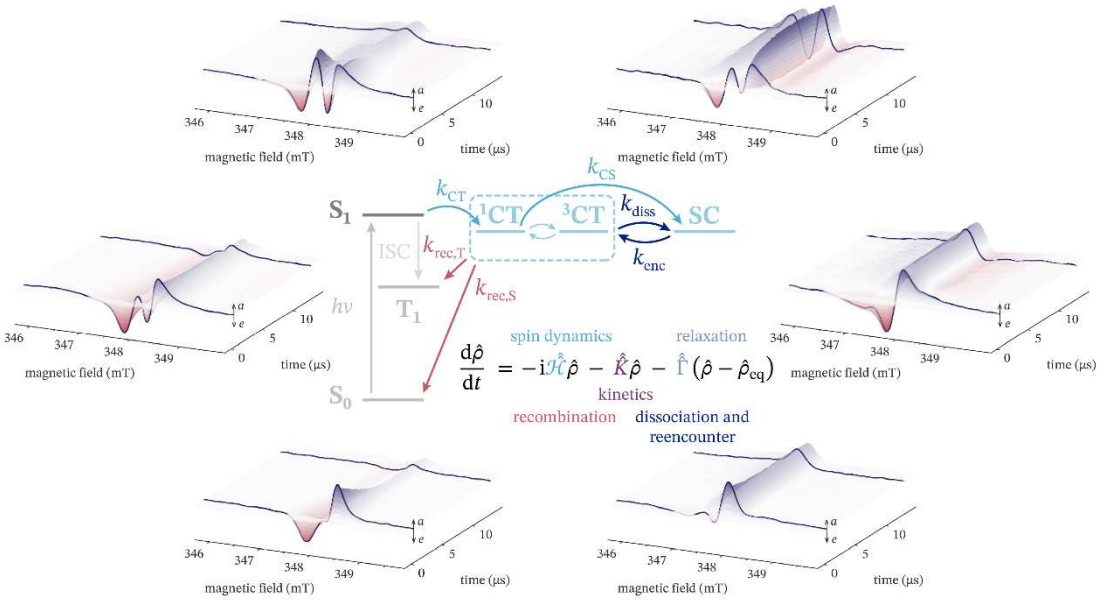
Spin dynamics of charge generation in organic photovoltaic and photocatalytic materials probed by ESR

Jack Palmer, Niall Curwen, Charlotte Hadfield, Claudia Tait

Department of Chemistry, University of Oxford, United Kingdom

Spin-correlated radical pairs are important intermediates in photoinduced charge separation processes across many biological and chemical systems, where spin selectivity governs both the initial state as well as the subsequent evolution [1]. Photoinduced charge separation is also at the core of photovoltaic energy conversion in organic donor:acceptor materials for organic solar cells, but the details of the charge separation process and the role of any charge-transfer states in these materials are currently still under debate [2].

EPR spectroscopy provides unique insights into this crucial initial step through the characterisation of photoinduced paramagnetic states and their spin polarisation. In this talk, I will discuss a series of transient EPR studies on organic systems for photovoltaic and photocatalytic energy conversion, highlighting a high degree of variability in the time-dependent evolution of spin polarisation across different donor:acceptor pairs. The evolution of the spin polarisation pattern encodes information on the formation and spin-dependent dynamics of the generated charged states. By combining experimental measurements with simulations of the full transient EPR surface using a model that incorporates both charge-transfer states and separated charges, we gain new mechanistic insights into the details of the charge generation process.



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Contributed Lecture

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

Edward R. Champness[1], Damyan S. Frantzov[1], Keagan D. Love[1], Ana Stuhec Kocijan[2], Kevin B. Henbest[1], Sebastian M. Kopp[3], Harry L. Anderson[1], Christiane R. Timmel[1], Gabriel Moise[1]

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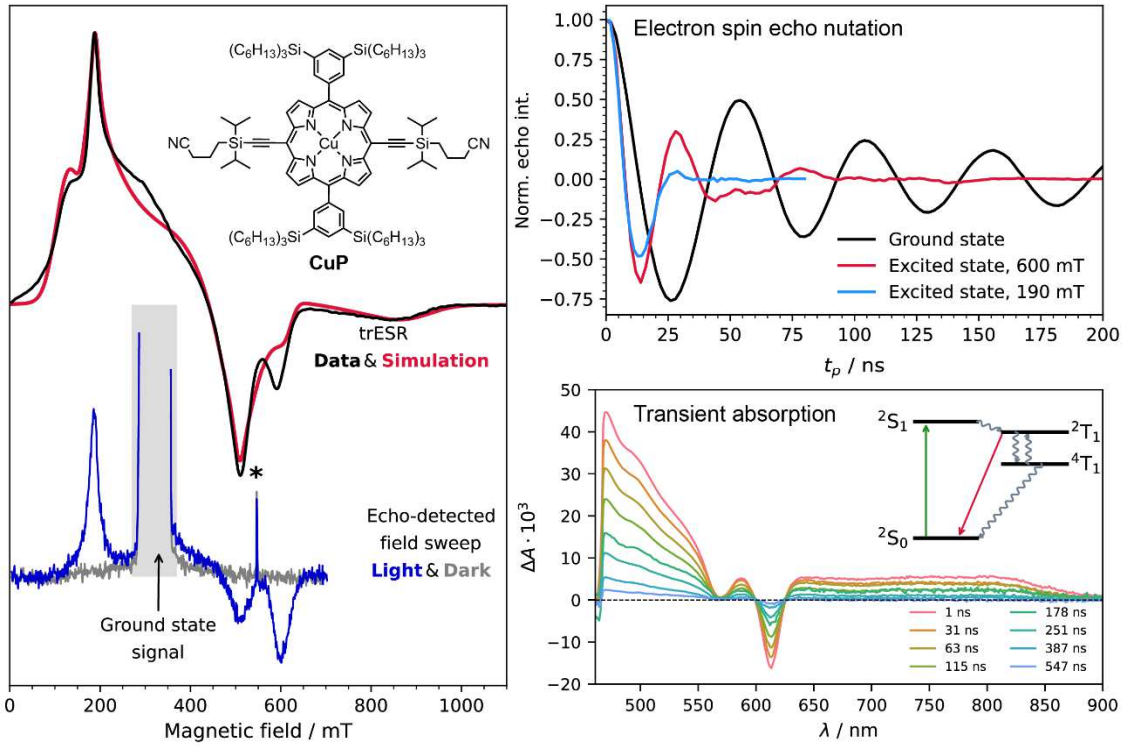
High-spin molecules are attractive candidates for quantum technologies due to their expanded spin manifolds enabling enhanced information density per qudit and potential error-correction capabilities [1–3]. Here, we report the generation and spectroscopic identification of a qudit candidate in the form of the photoexcited quartet state (S = 3/2) of a copper(II) porphyrin, CuP. Using transient absorption, time-resolved luminescence, pulse and transient electron spin resonance (trESR), we demonstrate the formation of a long-lived, spin-polarized excited quartet state. Nutation measurements provide direct evidence for the quartet multiplicity, while simulations with an effective quartet Hamiltonian reveal an unusually large zero-field splitting relative to the triplet excited states of diamagnetic porphyrins.



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Contributed Lecture

Photoexcited spin polarization in molecular systems from first principles

Yuki Kurashige[1,2,3]

[1]*Graduate School of Science, Kyoto University, Japan*
[2]*CREST/*[3]*FOREST, Japan Science and Technology Agency, Japan*

Electron spin polarization, a non-Boltzmann population distribution among spin sublevels, has been extensively studied in spin spectroscopy and related fields, including applications such as dynamic nuclear polarization (DNP) and optically detected magnetic resonance (ODMR). However, despite extensive studies of spin polarization phenomena, establishing a microscopic understanding that connects molecular electronic structures with spin polarization mechanisms remains an important challenge. Recent progress in quantum technologies has further motivated the exploration of molecular systems exhibiting controllable spin polarization.

For the rational development of such systems, theoretical approaches capable of analyzing and predicting photoinduced spin polarization directly from molecular electronic structures are becoming increasingly important. In this presentation, I will discuss our recent work on photoexcited spin polarization in molecular systems from a first-principles perspective, focusing on the prediction of (i) low-lying excited states with different spin multiplicities, (ii) molecular-frame zero-field splitting (ZFS) tensors, (iii) spin-selective intersystem crossing rate constants responsible for generating spin polarization, and (iv) theoretical descriptions of spin polarization lifetimes. Representative mechanisms and molecular examples are discussed, together with recent progress and remaining challenges in theoretical approaches for predicting spin polarization and relaxation from first principles.

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Invited Lecture

Enhanced ^{1}H and ^{19}F NMR Microwave-Free Optical Hyperpolarization in Liquids

Federico De Biasi[1], Lorenzo Franco[1], Marco Ruzzi[1], Gabriele Stevanato[1]*

[1] Department of Chemical Sciences, University of Padova, via Marzolo 1 35131 Padova, Italy

Optical dynamic nuclear polarization (oDNP) provides a microwave-free route to nuclear hyperpolarization in liquids but has so far remained limited by modest enhancements, poor photostability, and applicability essentially restricted to one-dimensional ^{1}H experiments.[1–3] Here, we show that porphyrin–BDPA pairs overcome these limitations. Under continuous illumination with LED (<0.5 W at the sample), a factor of two better than previous reports bulk-solvent ^{1}H enhancements are achieved at room temperature under static conditions, without detectable photodegradation. Beyond proton hyperpolarization, porphyrin–BDPA pairs enable the first liquid-state oDNP enhancement of ^{19}F nuclei and the first multidimensional oDNP-enhanced NMR experiment, demonstrated through a 2D ^{19}F COSY spectrum. The observation of positive ^{19}F enhancements suggests a significant scalar contribution to the polarization transfer mechanism. Together, these results establish porphyrin–BDPA pairs as a robust platform for multinuclear (^{1}H and ^{19}F) and multidimensional optical hyperpolarization, significantly broadening the scope of microwave-free DNP in liquids.

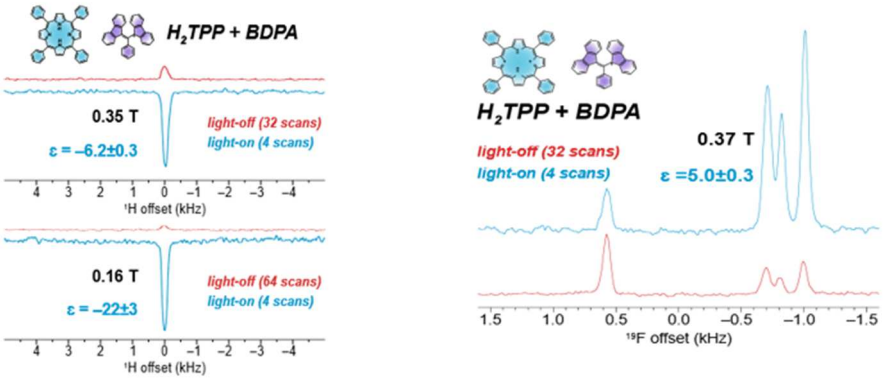

Figure 1: Solutions of 0.5 mM BDPA and 0.2 mM H_2TPP for negative ^{1}H optical DNP at 0.36 T and 0.16 T and for positive ^{19}F optical DNP at 0.37 T.

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Contributed Lecture

Accurate Large Spin Ensemble Simulations of High-Field and Fast-MAS Solid-State Dynamic Nuclear Polarization NMR

Enrico Bolognesi,[1,2] Ginevra Santioli,[1] Lorenzo Niccoli,[1] Marina Macchiagodena,[1] Frédéric A. Perras,[3] Anne Lesage,[4] Moreno Lelli[1,2]

[1] Center of Magnetic Resonance (CERM) and Dipartimento di Chimica, University of Florence, Via della Lastruccia 3, 50019 Sesto Fiorentino, Italy; [2]Consorzio Interuniversitario Risonanze Magnetiche Metalloproteine Paramagnetiche (CIRMMP) Via Luigi Sacconi 6, 50019 Sesto Fiorentino, Italy; [3]Ames Laboratory, U.S. DOE, Ames, Iowa 50011, USA; [4] Centre de RMN à Très Hauts Champs, Université de Lyon (CNRS/ENS Lyon/UCBL), 69100 Villeurbanne, France

Dynamic Nuclear Polarization (DNP) applied to MAS solid-state NMR has proved to be a valuable technique to enhance the sensitivity of more than two orders of magnitude at 9.4 T. Nevertheless, the performances at 9.4 T are strongly reduced at hight field like 18.8 T (800 MHz of ^{1}H), where the design of optimal Polarizing Agents (PAs) is still an open problem.

In 2020 we introduced novel, water soluble, dinitroxides biradicals, named TinyPols,[1] and last year further major improvements in the radical design were achieved: optimizing a molecular geometry promoting stronger electron-electron magnetic interaction and “antenna” side arms to promote an efficient radical-solvent interaction. In particular, M-TinyPol(OH)$_4$ showed enhancements up to about 200 even at 65 kHz of MAS frequency and 18.8 T.[2]

Here we present a detailed analysis of the DNP efficiency of these improved TinyPol biradicals, comparing the experimental enhancements with DNP computational simulations that support the experimental data. DNP simulations, performed with a hybrid QM DNP model[3] and Molecular Dynamics, makes it possible to follow the propagation of the polarization within the solvent matrix unravelling the roles of the antenna sidechains in promoting the hyperpolarization spin-diffusion (**Fig. 1**). The detailed comprehension of these processes opens the way to further progress in polarizing agent design, and it introduces a new tool for improving the efficiency of PAs.

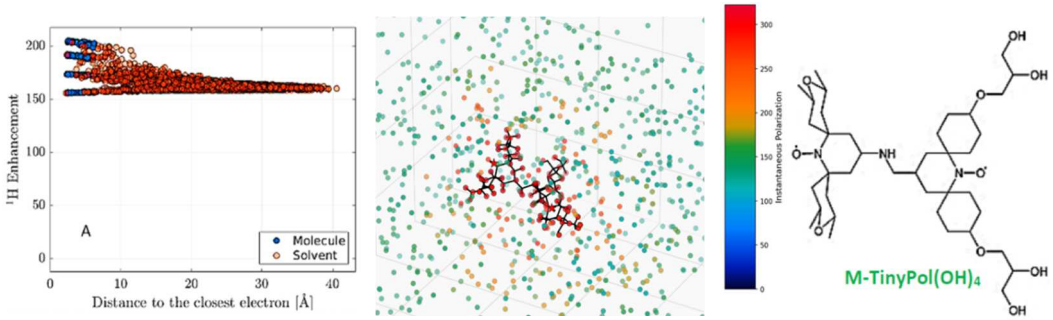

Fig. 1. DNP Large Spin Ensemble Simulations.

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[2] Niccoli, L.; et al. Chem. Sci. 2024, 15, 16582.
[3] Perras, F. A.; et al. J. Chem. Phys. 2022, 156, 124112.

Contributed Lecture

Optically Excited Molecules for DNP Applications

Yash Patel[1], Trent McHenry[1], Philip Weiss[1], Ilya Dergachev[1], Claudia E. Avalos[1]

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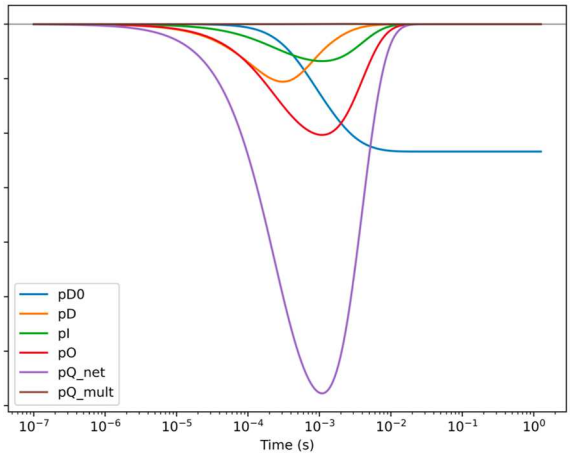
The ability to optically plarize spin states has applications in sensitive magnetic field detection as well as magnetic resonance signal enhancement. Photoexcited triplet states in organic chromophores or defects in solids can be combined with microwave irradiation to significantly enhance NMR signals [1]. Alternatively, in the absence of microwaves, the magnetic field can be tuned to specific matching conditions to allow for all optical nuclear spin polarization [2]. One may also take advantage of nuclear spin-dependent relaxation pathways which are present in select molecular systems (Chemically induced dynamic nuclear polarization, or CIDNP)[3]. What all of these approaches have in common is that the electronic transition rates often determine the ultimate 'cooling power'. How polarized, or how intializable are these systems under the best conditions? What are the molecular motifs that would maximize the ground-state spin polarization in a subset of these systems and within a reasonable amount of time? In this presentation I will discuss different classes of optically pumped molecular systems and I will discuss our recent efforts to determine which combination of molecular motifs lead to desirable electronic and magnetic coupling parameters to maximize multiplet and doublet electron spin polarization in chromophore-radical systems. We combine electronic structure calculations with experimental datasets and state-mixing dependent kinetic models to predict expected spin polarization in the excited and ground-state spin manifolds as a function of magnetic field and laser pump power.



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[3] De Biasi, F., Hope, M. A., Avalos, C. E., Karthikeyan, G., Casano, G., Mishra, A., ... & Emsley, L. (2023). Optically enhanced solid-state 1H NMR spectroscopy. Journal of the American Chemical Society, 145(27), 14874-14883.

Contributed Lecture

Towards the conductivity-magnetism interplay in hydroxylated ethylene-coupled tetrathiofulvalenes and nitronyl nitroxides for magnetoresistance applications

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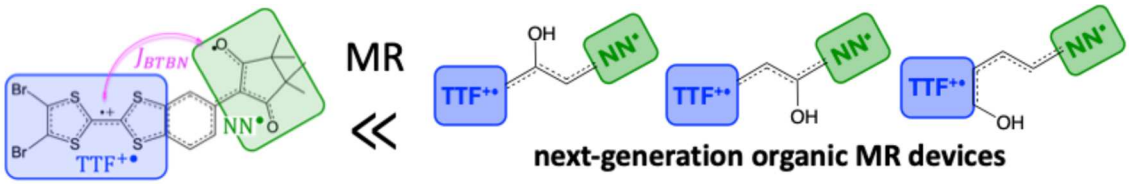
Organic materials are emerging as strong candidates for next-generation magnetoresistive technologies thanks to their molecular tunability, long spin-coherence times, and the possibility of co-optimizing charge mobility with magnetic-exchange interactions. In this computational work, we demonstrate how such co-optimization can be achieved using BTBN [1], a prototypical purely organic material exhibiting magnetoresistance (MR), as a reference system.

BTBN consists of covalently linked tetrathiafulvalene–nitronyl nitroxide (TTF–NN) dyads, where hole transport along TTF π-stacks is modulated by ferromagnetic (FM) exchange with the NN radicals, rendering hopping spin-dependent. Magnetic-field alignment of the NN spins therefore reduces resistance. We analyse three newly designed BTBN-derivatives with enhanced intramolecular FM coupling [2] and disclose the interplay between transport and magnetism. The use of both band-transport and hopping models provides cross-validated results. The derivatives show enhanced charge transport through larger hole mobilities and favourable injection alignment with gold electrodes, ensuring device compatibility. Their magnetic landscape remains weakly coupled yet field-tuneable, consistent with MR driven by spin ordering. Finally, the balance between hopping and spin interactions reveals that spin frustration can impede conduction, underscoring the key role of spin alignment. These materials showcase a clear route toward next-generation organic MR devices based on a rational design principle: the simultaneous optimization of charge mobility and intramolecular FM exchange. Overall, our study offers actionable guidance for experimental synthesis and validation.



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Contributed Lecture

EPR Study of charge transfer co-crystals Structure/Function Relationship

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Organic charge-transfer (CT) co-crystals exhibit unique electronic and magnetic properties depending on their molecular packing structures and aggregate states which exhibit a variety of novel properties through multicomponent synergistic and collective effects.
Ant/TCNQ and Naph/TCNB CT co-crystals have mixed stacking arrangements resulting in localized charges with long spin relaxation times T_m and T_1 as shown by EPR measurements. Fitting the relaxation times using second order exponential fit, gave two components with a ratio of 29: 71% for Ant/TCNQ and 40:60% for Naph/TCNB which was consistent with previous X-ray and solid-state NMR studies on the systems, indicating two species due to an in-plane molecular rotation within the crystal.
Computational study using CDFT of the D^+ or A^- geometry relaxation pave the way for obtaining a consistent experimental-theoretical picture. There is a clear-cut indication of the existence of localized stable spin-states within Ant/TCNQ and Naph/TCNB co-crystals, where the molecular structure is by far more complex than a simple D^+:A^-, in a 1:1 ratio, fundamental structure. Rather, the original view we here propose for the Ant/TCNQ and Naph/TCNB CT co-crystals, is that of a molecular architecture where isolated and localized charged A or D molecules are diluted within the crystal framework: a 3D crystal embedding isolated anions and cations, i.e. spins.
A further important outcome is the evidence that beyond the electronic properties of the single D and A partners, the role of the crystal structure and symmetry appears of fundamental importance. Since the HOMO-LUMO gap of the Ant/TCNQ is quite similar to that of the Naph/TCNB system, the EPR (number of spins) as well as the theoretical output are marked different. And indeed, the energy needed for the charge localization in the Ant/TCNQ system is lower compared to that of the Naph/TCNB, as it is also reflected by the much easier convergency of CDFT calculations for the former system. These results suggest a model where the CT co-crystal is composed of neutral packed molecules where localized charged ions are diluted, i.e. localized.
In addition, EPR study upon photoexcitation of Anthracene/TCNQ and Naph/TCNB co-crystals showed the formation of spin polarized radical-pair spectrum. Its EPR phase pattern indicates it is a triplet born radical pair.

Plenary Lecture

Nuclear hyperpolarization in synthetic donor–acceptor dyes by photochemically induced dynamic nuclear polarization

Lyndon Emsley

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École Polytechnique Fedérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Photochemically induced dynamic nuclear polarization (photo-CIDNP) is a hyperpolarization technique that can provide NMR signal enhancement factors of several orders of magnitude under continuous light irradiation.[1,2] In solids, we recently demonstrated that ^{1}H photo-CIDNP from synthetic donor–acceptor dyes can lead to the development of bulk nuclear spin polarization due to the action of spontaneous ^{1}H–^{1}H spin diffusion.[3,4] In these experiments, the optically active donor–acceptor systems act as nuclear spin polarizing agents under light irradiation, in full analogy with the stable organic biradicals typically used in magic angle spinning cross effect DNP NMR experiments. As such, ^{1}H photo-CIDNP could be used to establish a general light-induced hyperpolarization protocol to improve the sensitivity of solid-state NMR through the combined use of donor–acceptor dyes and optical irradiation.

Here, we show how the theory of photo-CIDNP can be used to underpin the key molecular features in such donor–acceptor systems that maximize the generation of bulk hyperpolarization in solids.[5] These results allow us to identify clear rational design strategies, paving the way to the development of second-generation polarizing agents for dye-sensitized NMR experiments.

[1] Bargon, *et al.*, *Z. Naturforsch. A* **1967**, 22, 1551.
[2] Cocivera, *J. Am. Chem. Soc.* **1968**, 90, 3261.
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[5] De Biasi, *et al.*, *J. Chem. Phys.* **2025***,* 163, 244113.

Invited Lecture

Studying the solid-state photo-CIDNP effect

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Our group has been studying the photo-CIDNP effect in solids for more than 25 years [1]. Initially, we investigated photosynthetic reaction centers to gain insights into their highly optimized spin-chemical mechanisms [2,3].

However, the possibilities for systematically modifying these systems are limited. LOV domains, which carry flavins as electron acceptors and utilize tryptophans as donors, are more flexible and also hyperpolarize the proton pool. We systematically investigated the distances and modified the donor from Trp to Tyr [4-6].

Using a LOV domain with Tyr as the donor, we were able to induce the effect for protons at 4.7 Tesla, thereby paving the way for new categories of experiments. We also will report on the use of artificial diads.

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[2] Yunmi Kim, Daniel Gräsing, A. Alia, Christian Wiebeler, Jörg Matysik, “Solid-state NMR analysis of the dynamics of cofactors in heliobacterial reaction centers”, J. Phys. Chem. B (2024) 128, 47, 11525-11545. DOI: 10.1021/acs.jpcb.4c04082.

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Invited Lecture

LC-Photo-CIDNP: A Gateway to Hypersensitive NMR Spectroscopy

Silvia Cavagnero, Anubhab Halder, Ji Ho Jeong, Samuel C. Carey, Ummay Mahfuza Shapla

Dept. of Chemistry, University of Wisconsin-Madison, Madison, WI 53706

Nuclear magnetic resonance spectroscopy is hampered by extremely low sensitivity. This presentation will explain how low-concentration photochemically induced dynamic nuclear polarization (LC-photo-CIDNP) is able to overcome this challenge by enabling ultra-rapid NMR data collection in solution across the low-micromolar-to-nanomolar concentration range. Recent conceptual advances and practical implementations of LC-photo-CIDNP to the nuclear-spin hyperpolarization of amino acids and proteins will be discussed, highlighting advantages and disadvantages. LC-photo-CIDNP data collection across a wide variety of applied magnetic fields and solution conditions (e.g., buffered solution and physiological relevant *milieux*) will be presented. In addition, we will highlight how through-bond and through-space polarization transfer further broadens the scope and applicability of LC-photo-CIDNP optically enhanced NMR. The above advantages pave the way to a variety of studies targeting the hypersensitive high-resolution analysis of molecular structure and dynamics *in situ,* in the context of biophysics, biotechnology and medicine.

Contributed Lecture

Chemical hydrodynamics of nuclear spin states

Anupama Acharya[1], Madhukar Said[2], Sylwia J. Barker[1,3], Marcel Utz[1,3], Bruno Linclau[1,2], Ilya Kuprov[4,1]

[1]*School of Chemistry and Chemical Engineering, University of Southampton, UK;*
[2]*Department of Organic and Macromolecular Chemistry, Ghent University, Belgium;*
[3]*Institute of Microstructure Technology, Karlsruhe Institute of Technology, Germany;*
[4]*Department of Chemical and Biological Physics, Weizmann Institute of Science, Israel.*

Fundamental equations of motion in quantum mechanics of isolated systems and ensembles are required (by causality and time translation invariance), to be linear with respect to state descriptors, such as wavefunctions and density matrices. However, the law of mass action in chemical kinetics and Navier-Stokes equations in hydrodynamics are not fundamental; they are statistical approximations, and therefore at liberty to be non-linear with respect to concentrations. This incompatibility creates insidious difficulties in theoretical descriptions of systems where quantum processes coexist with chemical kinetics and spatial transport, notably in spin chemistry, magnetic resonance imaging (MRI) of complex metabolic and hydrodynamic processes, and – our predicament here – nuclear magnetic resonance (NMR) in microfluidic chips. The problem involves a collision of approximations at the interface of classical and quantum physics broadly similar to the measurement paradox – although the concentration and the wavefunction amplitude square are both probability densities, one has a specific measurement outcome but the other does not.

For isolated spins and first-order reactions, this is a well-researched topic, but time evolution of complex nuclear spin systems in the presence of second-order kinetics, diffusion, and flow has so far remained intractable. In this communication, we report a theoretical formalism and a *Spinach* implementation for the full non-linear kinetics + magnetohydrodynamics case. The problem is a quantum mechanical generalisation of the Fokker-Planck formalism in which concentration is replaced by concentration-weighted density matrix and the evolution generator is both time- and state-dependent. Its efficient numerical implementation is difficult: dimensions of spatial dynamics generator matrices on finite grids can be large; when combined with the spin Hamiltonian of a typical metabolite, the composite evolution generators cannot even be stored; we solve the problem by keeping them in a polyadic format with buffered Kronecker products.

We apply the resulting methods and software to microfluidic chip NMR experiments in the simultaneous presence of diffusion, flow, and second-order chemical reactions. As an illustration, we use Diels-Alder cycloaddition of acrylonitrile to cyclopentadiene in a microfluidic NMR probe (a finite element model with thousands of Voronoi cells) with a spatially localised stripline radiofrequency coil.

https://doi.org/10.1126/sciadv.ady9103

Invited Lecture

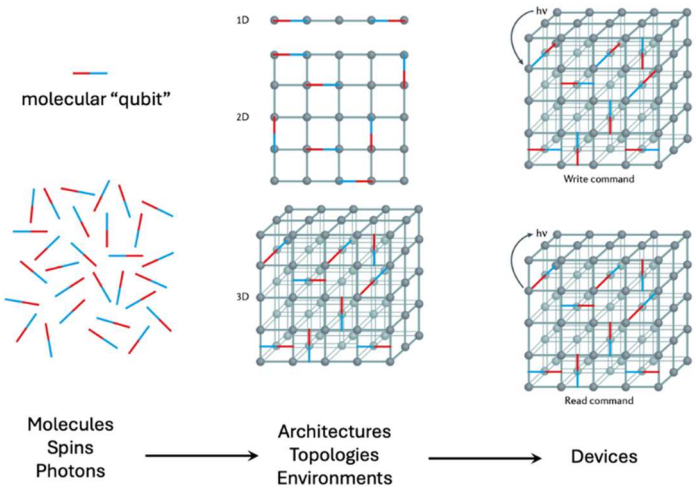
Two's Company, Three's Not a Crowd: Creation and Control of Multi-Spin Systems for Quantum Information Science Applications

Malcolm D. E. Forbes

Center for Photochemical Sciences
Department of Chemistry
Bowling Green State University

We are building, characterizing, and investigating novel systems for photoinduced electron spin polarization transfer that can be applied to quantum information science (QIS) technologies. We seek to understand how supramolecular architectures, topologies and local environments affect photoexcited state lifetimes, spin polarization magnitudes in nitroxide monoradicals, coherence integrity and coherence lifetimes in nitroxide biradicals, and overall chemical robustness in qubit candidates for potential QIS devices. We use optical spectroscopic methods and electron paramagnetic resonance (EPR) spectroscopy in steady-state, time-resolved (CW), and pulsed modes. Optimization of qubit candidates will have significant impact for applications in quantum computing, quantum sensing, and quantum communications.

There are many molecules currently proposed to be used in QIS systems, but there is a large knowledge gap regarding how electron spin information can be manipulated and transferred within and between larger molecular architectures such as single crystals, polymer matrices, and metal-organic frameworks. In less rigid systems such as micelles, reverse micelles and vesicles, molecular motion and/or confinement can also influence qubit qualities such as polarization magnitudes, relaxation times, or quantum interference effects. Small systematic variations in mobility, confinement, dilution, and orientation are being made to determine the most important parameters for optimal qubit performance. The results will help guide the transition from molecules to meta-architectures to realistic devices for future QIS applications.



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Contributed Lecture

From Electron to Nuclear Spins: Room-Temperature Optically Detected Coherent Control in Chemically Tuneable Molecular Qubits

Sarah K. Mann[1], Eoin Irving[1], Max Attwood,[2] Sam L. Bayliss[1]

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[2] Department of Materials and London Centre for Nanotechnology, Imperial College London, Prince Consort Road, London, UK.

Optically addressable molecular spins are emerging as a promising platform for quantum technologies, particularly sensing and imaging [1]. Their combination of chemical tunability with spin–optical interfaces for spin initialisation, coherent control and optical readout offers a route to tailor-made quantum sensing platforms.

Molecular design also provides a unique opportunity to engineer the nuclear-spin environment surrounding an optically addressable electron spin. Hybrid electron–nuclear spin systems combine the optical accessibility and sensing capabilities of electron spins with the long coherence times of nuclear spins, providing a potential route to memory-assisted quantum sensing. Realising this potential requires efficient initialisation, coherent control and readout of nuclear spins under practical operating conditions.

Building on our demonstrations of room-temperature optically detected coherent control of photoexcited electron spins in organic chromophores [2,3], I will show that coherent nuclear-spin control can be achieved and optically detected under ambient conditions. Using optically detected electron–nuclear double resonance (OD-ENDOR), we observe Rabi oscillations of coupled ^{14}N spins in a molecular qubit. Strong electron–nuclear hyperfine interactions enhance the nuclear-spin driving rate by several orders of magnitude, enabling rapid coherent manipulation despite the intrinsically weak magnetic moment of nuclear spins.

These results establish nuclear spins as a viable resource in optically addressable molecular qubits and demonstrate a pathway towards hybrid electron–nuclear architectures for memory-assisted quantum sensing at room temperature.

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Contributed Lecture

Single-Molecule-Scale Magnetic Resonance with Solid Spin Quantum Sensors

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With the rapid advancements in single-molecule science and the continuous development of new techniques, it has become possible to observe life processes at single-molecule level through multiple physical parameters windows. A promising approach is the use of solid spin defects in diamond and silicon carbide (SiC) as atomic sensors, enabling biocompatible detection of subtle changes in magnetic fields, electric fields, and temperature at the nanoscale. Here, we present our work utilizing nitrogen-vacancy (NV) centers in diamond to investigate the magnetic and thermal effects accompanying biomolecular activities [1]. We also introduce our recent results on two kinds of divacancy-related defects (PL5-6) in 4H-SiC using single-spin optically detected magnetic resonance spectroscopy, illustrating their potential as new quantum sensors working in near-infrared band [2].

[1] PNAS 122, e2509102122 (2025); Adv. Quantum Technol. 2300293 (2024); Science 347, 1135 (2015).
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Contributed Lecture

Engineering nuclear spin environments for molecular spin coherence: a multifrequency EPR study on luminescent perhalofluoro trityl radicals.

Naitik A. Panjwani[1], Johanna Schlögl[2], Geetika Naugain[2], Sebastian Riedel[2], Robert Bittl[1]

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[2] *Institut für Chemie und Biochemie – Anorganische Chemie, Freie Universität Berlin, 14195 Berlin, Germany*

The ability to optically initialize and read out spin states is central to emerging quantum technologies, including quantum sensing, communication, and information processing. Molecular systems are a promising quantum platform due to their reproducibility, chemical versatility, and precise geometric and spatial control achievable through accessible synthetic chemistry. Organic spin-radical semiconductors are particularly attractive in this regard as they can exhibit high luminescence [1, 2] and spin-dependent luminescence via high-spin states [3]. Recently, TTM-based diradicals have been shown to exhibit spin-dependent luminescence, coherent spin control at room temperature, and optical readout via optically detected magnetic resonance [4], establishing radical-based molecular systems as promising quantum platforms.

More recently, highly fluorinated trityl radicals [5] have emerged as a new class of luminescent open-shell molecules, displaying enhanced fluorescence quantum yields, longer luminescence lifetimes, improved photostability, and significantly altered local nuclear-spin environments compared with conventional chlorinated trityl radicals.

Building on these advances, we investigate how systematic tuning of the nuclear-spin environment through selective chlorine and bromine substitution in fluorinated trityl radicals influences electron spin coherence and relaxation. Using temperature-dependent multifrequency pulsed EPR spectroscopy together with hyperfine spectroscopic techniques, we probe the relationship between halogen substitution, hyperfine interactions, and spin coherence. These studies provide insight into the mechanisms governing decoherence in molecular radical systems and establish design principles for tailoring spin properties in future molecular quantum materials. Furthermore, such trityl radicals can exhibit chiroptical properties making them useful for chiral electronics.

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Contributed Lecture

Magnetic Field-dependent Isotope Effect in Tubulin Polymerization

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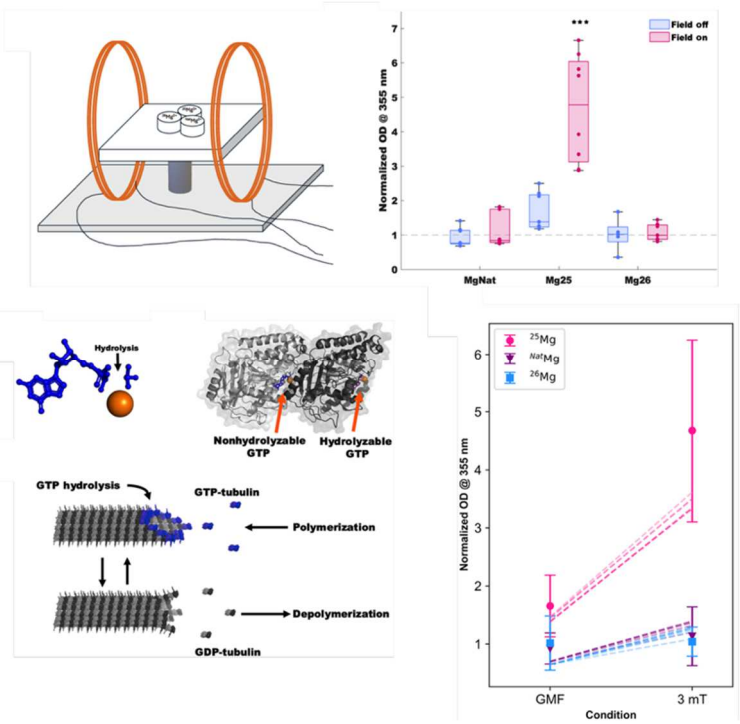
Weak magnetic field effects on biological systems are abundant and present a fundamental challenge: the energies involved fall far below thermal scales, ruling out classical explanations [1]. The radical pair mechanism (RPM) offers a quantum coherent explanation, whereby spin-selective recombination of transient radical pairs — governed by electron spin dynamics and modulated through hyperfine coupling to surrounding nuclear spins — can couple weak magnetic fields to chemical reaction outcomes [2]. Yet direct experimental evidence linking these nuclear spin contributions to macroscopic biological outcomes remains scarce. Here we report isotope-substitution experiments in which magnesium isotopes with differing nuclear spins (^{24}Mg, ^{25}Mg, ^{26}Mg) are used to probe spin-dependent chemistry during tubulin polymerization — a GTP-driven self-assembly process critically dependent on Mg^{2+} cofactors [3]. We observe isotope-dependent polymerization rates that are explicitly attributable to differences in nuclear spin, and show this effect is enhanced under an applied 3 mT static magnetic field. A radical pair model incorporating hyperfine coupling to the Mg nuclear spin achieves quantitative agreement with experimental observations. These findings establish tubulin as a tractable system testbed for RPM-based magnetosensitivity and implicate quantum spin dynamics in the regulation of cytoskeletal assembly.



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[2] PJ Hore, H Mouritsen, Annual review of biophysics 45 (1), 299-344, 2016
[3] H Zadeh-Haghighi, CR Siguenza, RP Smith, C Simon, TJA Craddock, Science Advances 12 (7), eady8317, 2026

Contributed Lecture

Spin Regulation Strategies for Enhancing Photoredox Catalysis

Li-Nan Zhou[1]*, Ming-Li Sun[1]

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Benefiting from low energy consumption and high atom economy, photoredox catalysis has become one of the core technologies for inert bond activation. Nevertheless, back electron transfer (BET) occurring in the singlet reaction channel seriously restricts the catalytic performance of organic photosensitizers. Despite the considerable progress achieved by catalyst optimization based on frontier orbital engineering over the past decades, it remains a formidable challenge.

To address this, we developed two innovative spin regulation approaches. First, a micellar microenvironment is constructed to promote the triplet reaction pathway in the photoreduction of inert (hetero)aryl chlorides. When coupled with an external magnetic field that suppresses spin conversion of radical ion pairs (RIPs), the forward efficiency is enhanced by up to 300%, with a maximum magnetic field effect of 160%. Second, Gd-DOTA is adopted as a spin catalyst solely to accelerate the singlet-to-triplet spin transition of RIPs in homogeneous organic solvents. This approach also effectively suppresses BET between radical ions derived from single electron transfer between the photocatalyst and the substrate. As a result, the reaction time required to reach a target conversion is shortened by 25-fold, delivering a spin catalysis effect of 70%.

Combining time-resolved spectroscopic techniques, including femtosecond transient absorption spectroscopy and nanosecond laser flash photolysis, with density functional theory calculations, we established a quantitative kinetic model and revealed the microscopic mechanism of spin regulation. This research puts forward an innovative physical regulation route for improving photoredox catalytic efficiency, and is promising to be further applied in complex organic synthesis.

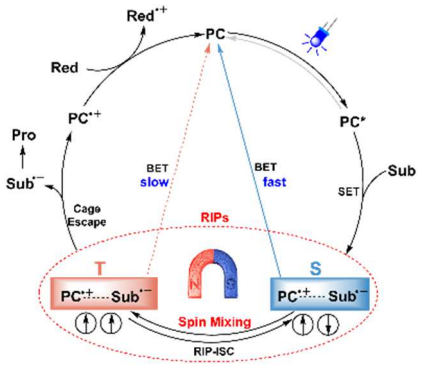

Fig. 1 Schematics of Kinetic Modulation of Photoredox Processes by an External Magnetic Field

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[2] Dong, Z.-Q.; Chen, C.-L.; Chen, L.-F.; Sun, M.-L.; Zhan, J.-Z.; Zhou, S.; Cao, L.-J.; Liu, J.-Y.; Bai, S.-M.; Jie, J.-L.; Su, H.-M.; Gao, S.; Zhou, L.-N. *Chem. Sci.* **2025,** 16, 17276–17286.

Invited Lecture

Electron and Nuclear Hyperpolarization in Blue-Light Activated Proteins: A Radical Pair Perspective

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Hyperpolarized nuclear spin and electron spin states frequently occur as short-lived intermediates following light excitation of proteins and artificial systems. These states can be probed directly or indirectly using time-resolved electron paramagnetic resonance (trEPR) and photo-induced dynamic nuclear polarization (photo-CIDNP) NMR, respectively. Their magnetic properties provide information about primary photophysical and photochemical processes. In this contribution, I will provide a brief update on our research from the past few years [1–9] and introduce some interesting new systems.

Acknowledgements: Many scientists in Freiburg[a], Hamburg[b] and Munich[c] contributed to the results presented in this contribution (in alphabetical order): Audrey Ayekoi[a], Adelbert Bacher[c], Johannes Berger[a], Jing Chen[a], Christopher Einholz[a], Markus Fischer[b], Boris Illarionov[b], Marco Ladwig[a], Maximilian Mayländer[a], Moustafa Okasha[a], Sabrina Panter[a], Sabine Richert[a] (⟶Ulm), Erik Schleicher[a], Anton Schmidt[a], and Jakob Wörner[a]. I owe them all a heartfelt thank you!

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Contributed Lecture

Nanosecond Structure of Radical Pair Intermediates from High-Frequency Quantum Oscillations. Elucidation of the $Q_A^{\bullet-}$ to Q_B Electron Transfer Step in Purple Bacterial Photosynthesis

Hideto Matsuoka[1], Gerhard Link[2], Ulrich Heinen[3], Oleg G. Poluektov[4], Lisa M. Utschig[4], Marion C. Thurnauer[4], Stefan Weber[2], Gerd Kothe[2*]

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[4]*Chemical Sciences and Engineering Division, Argonne National Laboratory, USA*

In this study, we first demonstrate the validity of our approach to deduce, from the anisotropy of quantum oscillations, the geometry of short-lived radical pair intermediates in photosynthesis. A global fit of a two-dimensional W-band (94 GHz) electron paramagnetic resonance (EPR) experiment provides the same global minimum values for the geometry of the A-branch radical pair $P_{700}^{\bullet+}A_{1A}^{\bullet-}$ in photosystem I as observed in a previous Q-band (34 GHz) EPR study yet with a significantly increased convergence rate of 62 % [1]. This shows that the underlying optimization problem is numerically well defined and its solution based on an efficient algorithm yields the correct pair geometry even at Q-band frequencies.

Second, with this information, we revisit our previous Q-band EPR study of the cofactor arrangement of $P_{865}^{\bullet+}Q_A^{\bullet-}$, the stabilized charge separated state in purple bacterial reaction centers. Analysis of calculated two-dimensional EPR data sets of $P_{865}^{\bullet+}Q_A^{\bullet-}$ reveals that the quantum oscillation technique is unaffected by a mirror ambiguity in disordered solids and thus can provide unambiguous solutions for all five Euler angles of the radical pair geometry [1]. This enables us to elucidate the $Q_A^{\bullet-}$ to Q_B electron transfer step in purple bacterial photosynthesis, the subject of controversial discussions for more than 25 years. We show that this electron transfer step involves a gating mechanism [2] requiring a 60° rotation of the head group of $Q_A^{\bullet-}$ in its binding pocket [1].

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Plenary Lecture

From Molecular Qubits to Quantum Sensors through Materials Chemistry

Nobuhiro Yanai[1]

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This century is witnessing a second quantum revolution, and quantum sensing represents an area in which chemists can make significant contributions. Chemically engineered molecular quantum sensors are compact and allow for precise control of their structure. Achieving quantum sensing requires more than precise control of quantum states at the molecular level; it is also crucial to organize qubits into molecular quantum *system* so that they function effectively in complex environments. In this talk, I will discuss materials chemistry approaches to molecular quantum sensors, focusing on their extension from biological systems to engineered materials.

We have recently enabled intracellular quantum sensing by developing a molecular quantum nanosensor (MoQN) [1]. By encapsulating atomically optimized molecular spin qubits within biocompatible nanocrystals, MoQNs achieve highly uniform spin energy levels and enable room-temperature optical detection of molecular spin states inside living cells. Compared with existing nanoscale quantum sensors, MoQNs exhibit superior uniformity, making absolute temperature sensing within cells possible—an achievement that has been challenging to realize with conventional platforms.

I will then show how molecular quantum sensing can be extended into chemically programmable materials. By incorporating photoactive chromophores as components of metal–organic frameworks (MOFs), these MOFs enable spatial organization and chemical accessibility of molecular qubits. This design allows quantum sensors whose spin coherence times respond to surrounding chemical species at room temperature [2,3]. Finally, I will discuss how controlled molecular assembly leads to multilevel quantum states (qudits). Through precise chromophore arrangement, singlet fission generates spin-correlated quintet triplet pairs with submicrosecond quantum coherence, expanding molecular quantum sensing beyond two-level systems [4,5].

Together, these examples illustrate how materials chemistry transforms molecular qubits from isolated spin systems into versatile sensing platforms that function across biological and materials environments.

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Invited Lecture

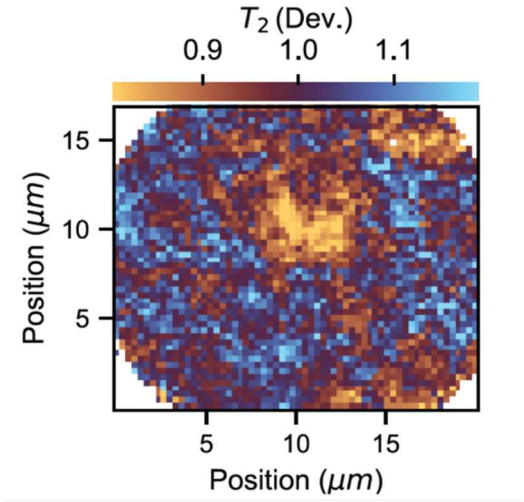
Spatially-resolved coherence of organic molecular spins at room-temperature

Adrian Mena[1], Nicholas P. Sloane[1], Max R. Bonengel[1], Cameron M. Gould[2], Scott A. Sulway[2], Dane R. McCamey[1]

[1]*School of Physics, University of New South Wales, Sydney, Australia*
[2] *School of Chemistry, University of New South Wales, Sydney, Australia*

Molecules offer a highly adaptable platform for quantum sensing, particularly as spin-bearing molecules can be chemically tuned and deployed in a range of formats, including crystals, thin films and solution. This flexibility makes them attractive for sensing architectures where proximity, spatial resolution and room-temperature operation are important.

In this talk, I will discuss how room-temperature optically detected coherent control [1] can be combined with microscopy to map the spatial variation of spin coherence in pentacene-doped p-terphenyl. Thin films provide practical advantages for sensing, including high doping ratios and nanometre-scale control of thickness, but they also introduce structural disorder. Micro- and nano-crystals, by contrast, can bring the spin sensor closer to the target while potentially preserving the coherence normally associated with more ordered solid-state systems. By imaging both thin films and micro-crystals, we show that thin films exhibit substantial spatial variation in contrast and coherence time, corresponding to approximately 7.6% variability in magnetic-field sensitivity (Figure 1). Micro-crystals show much lower sensitivity variability, around 1.3%, with no evidence of coherence loss toward the crystal edge. Finally, optically detected coherent control of a nano-crystal demonstrates that high-proximity molecular spin sensing can be achieved with minimal loss of performance relative to the bulk crystal, retaining a coherence time of 1.09 µs and a contrast of 25% [2].



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Contributed Lecture

Magnetic-Field-Dependent Delayed Fluorescence from Thermally Activated Reverse Charge Separation of Spin-Correlated Charge Separated States

Christoph Lambert[1], Tobias Groß[1], Paul Mentzel[1], Marco Holzapfel[1], Alexander Schmiedel[1], Ben Woodward[1], Nikita N. Lukzen[2], Ulrich E. Steiner[3]

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[2] *International Tomography Center and Novosibirsk State University, Novosibirsk, Russia 2*
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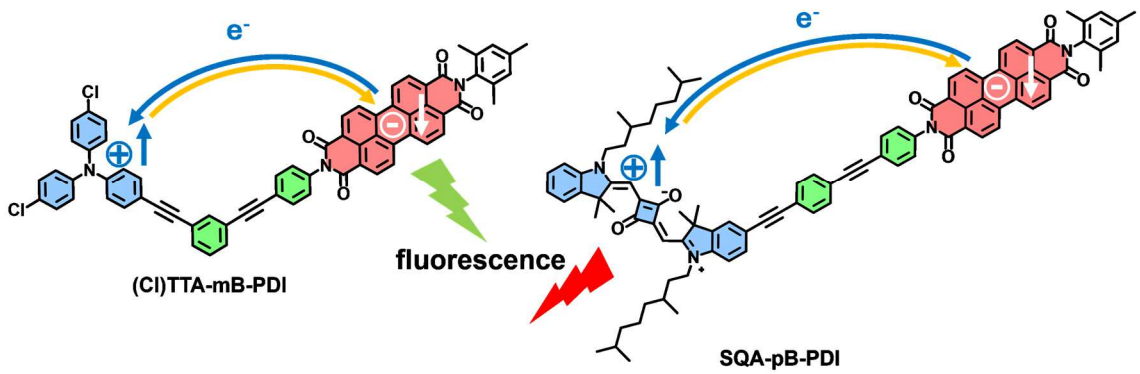
Thermally activated delayed fluorescence (TADF), involving reversible electron transfer between a fluorescing S_1 state and a magnetically responsive charge-separated (CS) state, constitutes a sensitive probe of the spin-chemical dynamics in the CS state as well as of the local magnetic molecular environment. With (Cl)TAA-mB-PDI and SQA-pB-PDI — featuring a Cl-substituted triarylamine ((Cl)TAA) or a squaraine unit as electron donors, meta-benzene (mB) or para-benzene (pB) bridges, and a perylene diimide (PDI) unit as electron acceptor — we introduce two novel triads with sufficiently small S_1–CS energy gaps to enable TADF. Their excited state properties were investigated by femtosecond and nanosecond time-resolved transient absorption spectroscopy as well as nanosecond time-resolved fluorescence spectroscopy at variable temperatures and in variable magnetic fields. The variable temperature data were used for a full kinetic and thermodynamic characterization of the reversible electron transfer in the excited state. The magnetic-field-dependent kinetic data were thoroughly analyzed using three models, progressing from a purely classical description to a fully quantum-mechanical treatment. These models explicitly incorporate the role of the S_1 state and show how the spin-dependent kinetics of the CS state govern the spin dependence of delayed fluorescence, establishing delayed fluorescence as a reliable indicator of the underlying spin dynamics.



Contributed Lecture

Spin-state-dependent photophysics of a spatially confined luminescent diradical and its magnetic modulation

Ryota Matsuoka[1], Yusuke Yoneda[2], Hikaru Kuramochi[1], Tomoaki Miura[3], Tadaaki Ikoma[3], Masaki Saigo[4], Takumi Ehara[4], Kiyoshi Miyata[4], Ken Onda[4], Shojiro Kimura[5], Tetsuro Kusamoto[1,6,7,8]

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[2]*Institute for Molecular Science, Japan*
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Luminescent organic radicals have attracted considerable attention due to their unusual photophysical properties such as the absence of heavy-atom effects, efficient carrier-to-photon conversion in electroluminescence, and spin-dependent excited-state dynamics. These properties stem from the doublet or higher multiplet spin states of radicals, which differ from those of conventional closed-shell molecules. In particular, multiple accessible spin states in luminescent multiradical systems hold great promise for future spin photonics applications including quantum information processing and sensing. Understanding the spin-state-dependent photophysics of molecular systems composed of multiple radical units is thus essential for establishing design principles for spin-correlated photofunctionality in multiradical systems.

We investigated the spin-state-dependent photophysical properties of a molecule containing two spatially proximate luminescent radicals (diradical **1**, Fig. 1)[1,2]. This molecule is an ideal model system for understanding detailed photophysical processes of luminescent radical dimers with weak spin–spin interactions. We demonstrate magnetic field effects on luminescence of **1** at cryogenic temperatures, and present a comprehensive spectroscopic characterization of the excited-state dynamics and electronic character of the singlet and triplet excited states for **1**.

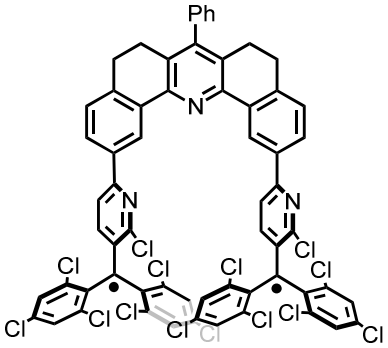

Fig. 1. Chemical structure of luminescent diradical **1**.

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Invited Lecture

Molecular Spins and Chirality as Resources for Quantum Technologies

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We are now witnessing the so-called Second Quantum Revolution and Quantum Technologies promise to open new possibilities in fields ranging from computing to secure communications. Molecular Spins [1] provide an interesting tool for quantum technologies. In fact, they are often characterized by a sizeable number of low-energy states that can be coherently manipulated, thus opening the possibility to use them to encode qudits. This offers the possibility of embedding quantum error correction into single molecules [1,2] and to improve the efficiency of quantum simulations [3,4].

In this presentation, I will review recent results on molecular spins as resources for quantum technologies. I will discuss the first implementation of the Quantum Fourier Transform using molecular qudits [5], achieved by embedding a full-refocusing protocol for qudits into the QFT sequence, thus enabling high-fidelity computation. I will then show that the temperature-resilient Chiral-Induced Spin Selectivity phenomenon persists down to the molecular scale [6,7] and can be exploited to significantly increase the operating temperature of molecular spin qubits [8]. Finally, I will discuss how electron–electron and electron–vibrational interactions provide key ingredients for understanding CISS [9].

These researches received financial support from the European Union's ERC-Synergy project CASTLE (proj. n. 101071533); from European Union – NextGenerationEU, PNRR MUR project PE0000023-NQSTI; from Novo Nordisk foundation grant NNF21OC0070832.

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Invited Lecture

Chirality-Induced Spin Selectivity in Photoinduced Charge-Separations of Cryptochrome for Magnetoreception

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[2] *Graduate School of Science, Kobe University*

The discovery of chirallity-induced spin selectivity (CISS) has introduced a new dimension to the study of spin phenomena in soft matter and biological systems. CISS refers to the remarkable ability of chiral molecules to preferentially transmit electrons or holes of one spin orientation, producing significant spin polarization even at ambient temperatures. However, the relevance of CISS to biological electron transfer, and in particular to radical pair-based magnetosensitivity, remains largely unexplored. Time-resolved electron paramagnetic resonance (TREPR) spectroscopy offers a powerful means of addressing these questions,(1) as it provides direct access to electron spin polarization dynamics with angular resolution. Previous findings suggest that structural and dynamical aspects of the protein matrix are intimately linked to magnetosensitivity on the spin-selective recombination.(2)

In this work, we extend TREPR analysis to investigate in detail the anisotropy of electron spin polarization in photoinduced charge-separated states of cryptochrome of WT *XlCry*-DASH (Figure 1). Specifically, we examine the influence of CISS on spin polarization and its interplay with protein conformational changes associated with long-range electron transfer. By combining insights from spin chemistry, chiral electron transport, and protein structural dynamics, this study aims to clarify the role of CISS in cryptochrome photochemistry and to provide new understanding of the quantum physical principles for the anisotropic signal transduction underlying biological magnetoreception.

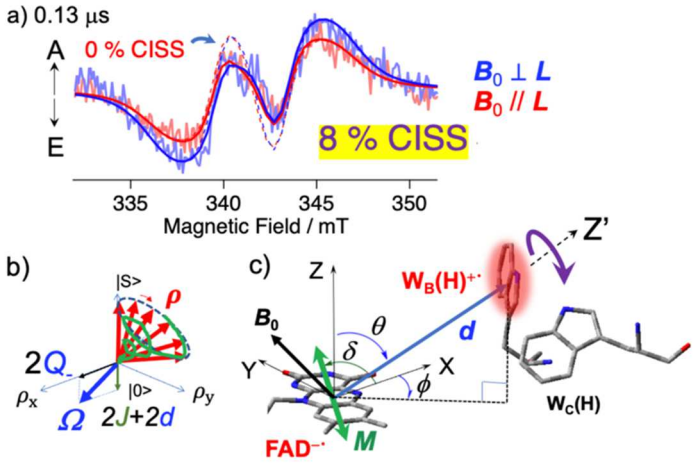

Figure 1. a): Magnetophotoselection effect of the TREPR spectra of $FAD^{-\bullet}\cdots W_B(H)^{+\bullet}$ at 120 K with $\mathbf{B}_0 \perp \mathbf{L}$ (blue) and $\mathbf{B}_0$ // **L** (red) obtained by polarized 450 nm laser irradiations of WT XlCry-DASH at 120 K.

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Invited Lecture

New Approaches for Studying Magnetic Field Effects in Radical pair Chemistry

Stuart R Mackenzie

University of Oxford, Chemistry Research Laboratory, OX1 3TA

Cryptochrome 4a has emerged as a leading contender for the magnetosensing molecule in migratory birds.[1] Within this hypothesis, photoexcitation of a bound flavin adenine dinucleotide (FAD) triggers an electron transfer cascade along a tryptophan chain resulting in formation of a spatially separated spin-correlated radical pair. Competitive singlet-triplet mixing, radical recombination and radical (de-/)protonation leads to magnetic field effects which are reflected in the concentrations of long-lived radicals produced.

The magnetosensitive photochemistry of cryptochromes is complex and a clear understanding typically requires a comprehensive range of spectroscopic techniques ranging from electron paramagnetic resonance to ultrafast optical spectroscopy.[2] Over the last decade we have developed a range of sensitive optical cavity and fluorescence-based techniques optimised for magnetic field effect detection in proteins.

This talk will focus on recent advances in spectroscopic technique development designed to combine sensitivity with high time resolution and broadband visible detection. Examples will focus on avian cryptochromes and their mutants [3] to better understand the role of tyrosine residues and isotopically enriched FAD as a test of the radical pair mechanism.

Expression of cryptochromes with bound flavin remains a considerable challenge and we continue to miniaturise our instrumentation to make best use of precious samples. To this end, we will also demonstrate fluorescence detection of magnetic field effects in microfluidic droplets including our first results on flavoproteins.

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Invited Lecture

Magnetic Field Effect Microscopy of Radical Pairs in Biological Systems

Noboru Ikeya[1], Shogo Ono[1], Mio Omi[1], Jonathan R. Woodward[1]

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The radical pair mechanism currently represents the most widely accepted hypothesis to explain the magnetic compass ability of migratory birds [1] as well as magnetoreception in many other animals, and represents a unique example of a biological capability enabled exclusively by virtue of a coherent quantum mechanical process. However, direct evidence for radical pairs undergoing magnetic field sensitive reactions in living systems remains sparse.

Photochemically generated radical pairs and magnetic field effects thereon have been extensively studied experimentally in chemical systems. In order to confirm and fully investigate their role in biology, we have developed microspectroscopic methods based on established spectroscopic techniques to monitor photochemical reactions proceeding through radical pair intermediates with sufficient time resolution, spatial resolution and sensitivity in real time, to observe species at cellular level concentrations on submicron length scales.

Here we present our studies on radical pairs exploiting steady state and time-resolved transient optical absorption and fluorescence microscopy for a wide range of radical pair reaction environments from aqueous solution to living cells. Transient optical absorption methods provide direct spectroscopic and time-resolved information about the radical pairs. To achieve time-resolved fluorescence microscopy with comparable information content, but with much greater sensitivity, we have developed Pump Probe (PP) and Pump Field Probe (PFP) based fluorescence methods [2] which give information which usefully complements that obtained from absorption-based methods. Steady-state methods then provide additional information about total reaction cycles containing slow processes. We focus on magnetically sensitive radical pair processes taking place in biologically relevant systems including purified proteins and living cells. In particular we will present details on our studies of magnetic field effects on cellular autofluorescence [3] which provide direct evidence for the radical pair mechanism operating in living cells, and expand to our most recent findings which demonstrate substantial magnetic field responses in unmodified bacteria.

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Plenary Lecture

Engineering molecular-spin-based quantum technologies

Arzhang Ardavan

Department of Physics, University of Oxford

Since soon after the recognition that quantum spins in condensed matter may offer useful physical embodiments of qubits, molecular magnets have been pursued as quantum technology platforms because synthetic chemistry offers engineerable spin Hamiltonians and, in principle, scalable assembly strategies [1,2].

An example that is relevant to a central challenge in the development of scalable quantum computers is the potential for a molecular spin system to be designed to expose the degrees of freedom required to implement quantum error correction protocols in a hardware-efficient way [3]. Using electron-nuclear double resonance, we have explored experimentally the implementation of a logical qubit encoded on the four states of a I = 3/2 nuclear spin hyperfine-coupled to a S = 1/2 electron spin qubit; the encoding protects against the dominant decoherence mechanism in such systems, fluctuations of the quantizing magnetic field. We have studied the dynamics of the encoded state both under a controlled application of the fluctuation and under natural decoherence processes [4]. Our results confirm the potential of these proposals for practical fault tolerant quantum memories.

However, a full implementation of this and related schemes requires projective measurement of the spin qubit, which, generally, remains challenging for molecular candidate systems. Addressing this, we have investigated the potential offered by DNA as an assembly technology for integrating molecular quantum components into electrical devices with high yield and high reproducibility [5].

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Invited Lecture

From diamond defects to protein-based qubit sensors

Peter Maurer[1]

[1]*University of Chicago, Chicago US*

Quantum metrology enables some of the world's most sensitive measurements with potentially far-reaching applications in the life sciences. Although the ultrahigh sensitivity of qubit sensors has sparked the imagination of researchers, implementing them in actual devices that enable monitoring cellular processes or detecting diseases remains largely elusive. Overcoming the limitations that hinder the broader application of quantum technology in the life sciences requires advances in both fundamental science and engineering. In this talk, I will discuss new strategies that combine quantum engineering and molecular biology to develop a new generation of quantum sensors that can be readily integrated with biological systems. My discussion will start with the development of a novel biocompatible surface functionalization architecture for highly coherent diamond crystals. I will then continue with discussing a new approach to engineering spin coherence in core-shell structured diamond particles, which can be readily chemically modified and delivered to intact biological systems. Finally, I will depart from established diamond sensors and introduce an entirely new class of biological qubits based on optically-addressable spins in fluorescent proteins. These protein-qubits have coherence times and optical readout comparable to solid-state defects, but are only 3 nm in diameter and genetically encodable. The unifying theme of these advances is the convergence of techniques from quantum engineering and molecular biology. Specific applications of the developed sensing platforms to questions in the life sciences will be discussed throughout this talk.

Contributed Lecture

Light-induced behaviour of Cr-based antiferromagnetically-coupled heterometallic systems

Susanna Ciuti,[1] Selena J. Lockyer,[1] Arianna Cantarella,[2,3] D. K. Andrea Phan Huu,[2] Alessandro Chiesa,[2,3,4] Grigore A. Timco,[1] Adam Brookfield,[1] Derren J. Heyes,[5] Eric J. L. McInnes,[1] Stefano Carretta,[2,3,4] Richard E. P. Winpenny,[1] Alice M. Bowen[1]

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[2] *Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, Parma, Italy*
[3] *INFN-Sezione di Milano-Bicocca, gruppo collegato di Parma, Parma, Italy*
[4] *UdR Parma, INSTM, Parma, Italy*
[5] *Manchester Institute of Biotechnology, University of Manchester, Manchester, UK*

{Cr_7Ni} antiferromagnetically coupled rings (Figure 1a) have been long investigated as potential molecular qubits, as two-level systems with agreeable phase memory times for application of gate operations [1]. These systems have shown to be flexible tools for building multi-qubit architectures [2] and have been successfully employed in supramolecular constructs with redox-switchable linkers [3]. To work towards the application of light-switchable molecular quantum gates, we present an investigation of the effect of laser excitation in the visible range on different Cr-Ni systems via time-resolved Electron Paramagnetic Resonance spectroscopy (trEPR) experiments. We observe unexpected strong, long-lived emissive trEPR signals (Figure 1b) and we interpret them as resulting from the inversion of the doublet ground state polarization of the Cr-Ni systems, employing a theoretical model to discuss a potential mechanism based on selective relaxation pathways and the permanent exchange interaction.

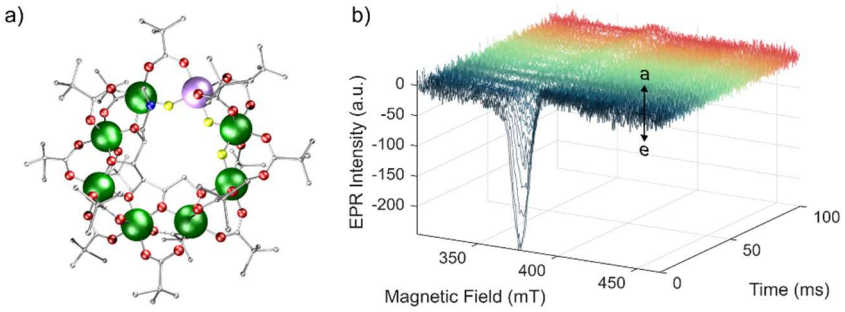

Figure 1: a) Crystal structure and b) X-band trEPR spectrum at 3 K of a {Cr_7Ni} ring in a toluene:dichloromethane frozen solution, after excitation at 560 nm.

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Contributed Lecture

Electric-field control of spin-exchange couplings in organic diradicals and 2D covalent organic frameworks

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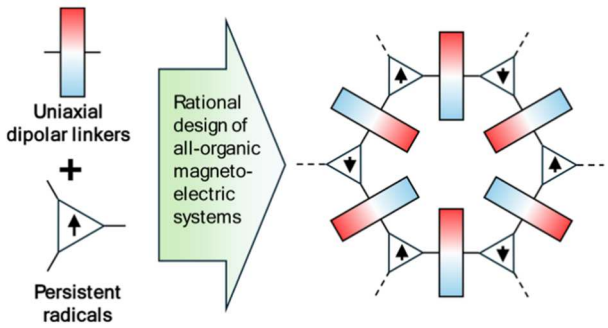
Development of technologically promising magnetoelectric materials, in which magnetic properties can be controlled by electric fields (E-fields), has largely focused on inorganic systems [1]. Here, we propose a strategy for modulating magnetic exchange coupling (*J*) in purely organic systems through experimentally realizable E-fields. Our strategy builds upon two established concepts: (i) E-field-induced conformational twisting of dipolar organic axial linkers [2] and (ii) control of *J* via mechanical or thermally driven conformational changes in organic diradicals [3].

Using density functional theory calculations, we investigate the effects of applied E-fields on diradicals with two coplanar spin-carrying trioxotriangulene (TOT) radicals connected by dipolar aryl linkers. Our results show that E-fields induce significant conformational changes in the linkers (twisting) that alters π-conjugation and, in turn, the magnetic *J* coupling between TOT radicals. In-plane E-fields twist the linkers toward the plane of the radicals, enhancing π- conjugation and increasing AFM coupling. Out-of-plane E-fields induce more orthogonal linker conformations and decrease the coupling strength. Significant and measurable cumulative changes in *J* of up to 3.9 meV (31 cm^{-1}) can be achieved by using in-plane and out-of-plane E-fields of up to 0.5 V/Å [4]. Calculations on a 2D covalent organic framework based on a network of TOT radicals and dipolar linkers confirm that this approach is also viable for extended systems [4]. Overall, these results establish a proof of concept for the design of all-organic magnetoelectric materials.



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Invited Lecture

Triplet Diradical Optical-Spin Interfaces for Quantum Sensing

S. M. Kopp[1], S. Nakamura[1], Y. Poh[2], K. R. Peinkofer[1], B. T. Phelan[1], J. Yuen-Zhou[2], J. R. Palmer[1], P.A. Watts[1], M. D. Krzyaniak[1], M. R. Wasielewski[1]

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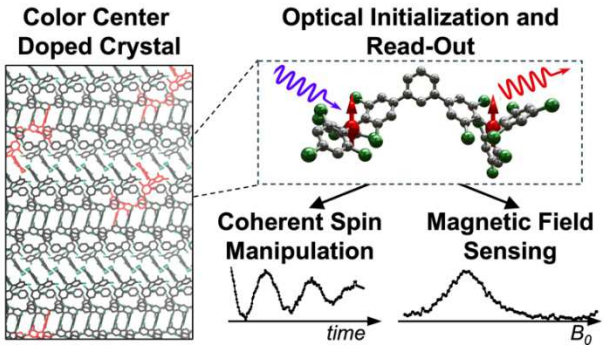
Molecular electron spins have emerged as versatile quantum bits (qubits) with wide ranging applications in quantum computing, sensing, and coherent communications at the nanoscale. These applications take advantage of the ability of chemical synthesis to 1) create specific structures with atomic scale spatial control; 2) tailor the magnetic, optical, and electronic properties of the qubits; and 3) construct large-scale ordered arrays of qubits via crystal growth and self-assembly. In order to take further advantage of the tunability of molecular qubits, optical-spin interfaces must be developed to permit addressing and readout of spin information.

Molecular optical-spin interfaces are promising alternatives to solid state defects such as nitrogen vacancy centers in diamond for quantum sensing applications. We will report on molecular optical-spin interfaces based on luminescent stable organic triplet diradicals. Optical spin polarization of the triplet state is achieved by spin-selective excited-state intersystem crossing. These systems are characterized by a combination of time-resolved optical, EPR, and ODMR spectroscopies. We demonstrate coherent microwave control of the spin-polarized ground state populations and coherences using optically detected Rabi nutations, Hahn echo formation, and echo decay measurements. 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.



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Invited Lecture

Using Spin Polarization and Transient EPR to Study Charge Separation in Al(III) Porphyrin Homodimer – Fullerene Supramolecular Assemblies

Art van der Est[1], Stefan Charon[2], Niloofar Zarrabi[2], Jatan K. Sharma[3], Peyton Ellis[2], Paul A. Karr[4], Francis D'Souza[3] and Prashanth Poddutoori[2]

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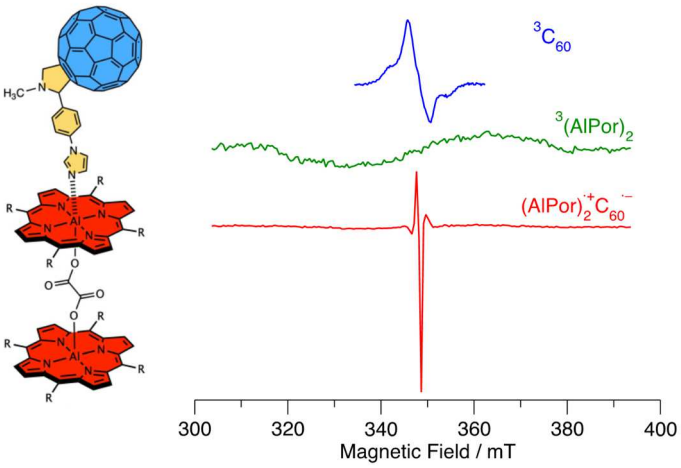
Aluminum(III) porphyrins exhibit properties that make them ideal candidates for mimicks of the primary donors in photosynthetic reaction centers. Their ability to form axial covalent and coordination bonds makes it possible to construct co-facial dimeric structures that mirror the geometry of the special pair dimers found in reaction centers. Moreover, the axial bonding ability can also be used to functionalize these dimers with electron acceptors and donors to create complexes that mimic the photosynthetic electron transfer chain.

Here, we report on a homodimer system comprised of two Al(III)-porphyrins covalently bound in a face-to-face arrangement by an axial oxalate di-ester bridge [1]. Using coordination of an appended imidazole to the Al center, C_{60} can be bound to the dimer to create a self-assembled donor-acceptor complex. In the soft glass phase and in liquid solution when solvent reorganization is possible, the spin polarized transient EPR spectra of the dimer-fullerene complex show that a high yield of light induced charge separation occurs. At lower temperature in the rigid glass, only the spectra of the porphyrin and C_{60} triplet states are observed. However, analysis of the spin polarization pattern of the porphyrin triplet state shows that it is formed partly by radical pair recombination. This suggests that in the absence of solvent reorganization, the radical pair state is higher in energy than the porphyrin triplet. Both the yield and lifetime of the charge separation in soft toluene glass are longer than in similar complexes in which the donor is a porphyrin monomer, illustrating the stabilization achieved with a dimeric donor.



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Contributed Lecture

Systematics of Photoinduced Spin Dynamics in Rigid Chromophore–Radical Compounds

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Photoexcitation of rigid chromophore–radical compounds leads to population of metastable states whose spin dynamics is governed by three principal stages: initial intersystem crossing, doublet–quartet evolution, and relaxation to the ground state. These processes determine the formation and redistribution of spin populations.

The spectral features of such systems can be classified on the basis of transient EPR spectra in terms of weakly and strongly coupled triplet–doublet regimes. Apart from these limiting cases, some chromophore–radical compounds may exhibit two additional spectroscopic regimes at intermediate exchange coupling. The first is the D/J-dominant regime, in which the zero-field splitting is comparable to or larger than the exchange interaction, leading to mixing of the doublet and quartet states. The second is the regime of anticrossings of doublet and quartet sublevels, when the exchange and Zeeman energies become comparable and their balance strongly affects the intensities and signs of the central lines in the transient EPR spectrum.

The presentation will discuss the systematics of these phenomena in terms of the spectral features and kinetic behavior observed by transient EPR spectroscopy.

The work is supported by a grant provided by the Academy of Sciences of the Republic of Tatarstan to higher education institutions, scientific and other organizations, to support human resources development plans in the part concerning the stimulation of their scientific and scientific-pedagogical staff to defend Doctor of Science dissertations and to carry out research work.

Contributed Lecture

Designing radicals for upconversion – substitution effects of rylene chromophores

Kieran Richards[1], Yoshika Takewaki[2], Jingkun Shen[3], Timothy J. H. Hele[3], Tetsuro Kusamoto[2], Emrys W. Evans[1]

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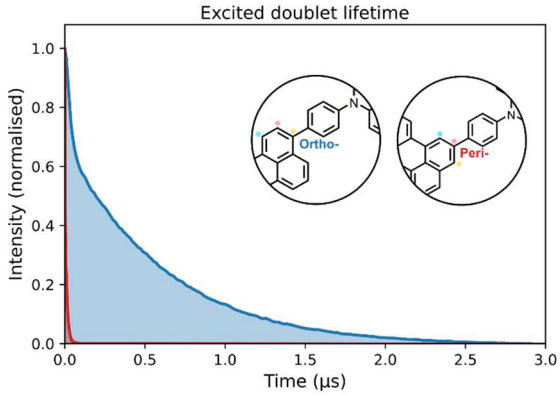
[2] *University of Osaka, Osaka, Japan,*
[3] *University College London, London, UK.*

Organic luminescent radicals have seen growing interest for use in photochemical upconversion, where energy transfer to the annihilator occurs directly from doublet state, bypassing the energy-losses seen for closed-shell sensitisers.[1,2,3] Despite this, they fall short of their organometallic counterparts due to their short excited-state lifetimes – a key parameter in bimolecular upconversion. We recently showed that conjugation of a spin-doublet radical sensitiser with a typical singlet-triplet annihilator chromophore (acene derivative) could enhance its lifetime (>250 ns) and therefore the upconversion quantum yield.[4] Here we investigate how subtle changes in molecular configuration between components can lead to dramatic changes in upconversion-relevant properties, such as 10 fold increase in fluorescence quantum yield and 60 fold increase in emission lifetime from doublet-quartet excited-state manifold.

The molecules investigated in this study are derived from PyBTM'-TPA and show near-infrared absorption >750 nm, useful for biological sensing.[5] Rylene linkage to these radicals is set by ortho- or peri- substitution. For the ortho- sample, upconversion is seen from excitation at 785 nm, with 1.12 eV shift. Temperature dependence and transient-absorption kinetic studies are used to explore the evolution of the rylene-localised triplet state and its role in upconversion. Transfer of the spin polarised triplet state from radical to annihilator is investigated using ESR and magnetic field effects. From this we suggest design rules that minimise internal losses and maximise the lifetime and quantum yield for photochemical upconversion.



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Contributed Lecture

Toward Blue Emission in Radical emitters: TEMPO radical coupled to TADF and INVEST Scaffolds

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[2]Laboratory for Chemistry of Novel Materials, University of Mons, Place du Parc, 20, 7000 Mons, Belgium.

Organic radicals have emerged as promising emitters for organic light-emitting diodes (OLED) because they allow bypassing the unfavorable 1:3 singlet-triplet spin statistics encountered for conventional closed-shell molecules by emitting light from the spin-allowed first doublet excited state (D_1), enabling internal quantum efficiency (IQE) of up to 100% [1]. Yet, the color palette of these OLED radical emitters was limited to the red/near-infrared emission regions, and they also suffered from color purity issues due to the pronounced charge transfer (CT) character of the emissive D_1 state. This limitation was recently overcome by covalently linking a non-emissive stable TEMPO (2,2,6,6-tetrametil-piperidi-1-nil)oxi) radical to a donor-acceptor (D-A) thermally activated delayed fluorescence (TADF) compound that shifted emission to green [2]. However, blue-emitting radicals remain scarce, and design rules are needed. Motivated by these experimental findings and seeking potential green/blue radical emitters, we performed quantum chemical calculations on TEMPO derivatives covalently linked to well-known closed-shell emitters: DMAC-NAI, a D-A TADF compound, DABNA-1, a multi-resonance TADF (MR-TADF) emitter, and Heptazine, an inverted singlet-triplet gap (INVEST) molecule. These compounds exhibit a peculiar electronic structure where the triplet state localized on the chromophore couples with the radical spin to form two dark states, namely trip-doublet ($^2[D_0T_1]$) and trip-quartet states ($^4[D_0T_1]$). The energy splitting is typically small (~ k_bT) and the signal of the exchange coupling (J) indicates ferromagnetic (J > 0) or antiferromagnetic (J < 0) interactions. Across all systems, multireference QD-NEVPT2 suggests an antiferromagnetic coupling, consistent with NEVPT4 prediction, despite NEVPT4 predicting larger J coupling. Relative to their closed-shell counterparts, the singlet-triplet energy gap (ΔE_{ST}) is larger for DMAC-NAI-TEMPO and Heptazine-TEMPO, but smaller for DABNA1-TEMPO. Another interesting feature is that the oscillator strength increases by around one order of magnitude for DMAC-NAI-TEMPO and Heptazine-TEMPO compared to their closed-shell analogues, while it remains strong for DABNA1-TEMPO. This study opens up new avenues and provides new insights into the design of radical-chromophore compounds with green/blue emission.

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Invited Lecture

Coherent Spin dynamics and Low Field Effect

Yoshitoshi Matsushita[1], Yuya Nakamura[1], U. E. Steiner[2], Christoph Lambert[3], Kiminori Maeda[1]

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[2]*Department of Chemistry, University of Konstanz, Universitätsstraße 10, 78464 Konstanz, Germany*
[3]*Institut für Organische Chemie, University of Würzburg, Am Hubland, 97074 Würzburg, Germany*

When investigating the dynamics of long-lived radical pairs with time resolved spectroscopy as transient absorption (TA), typical decay kinetics is multi exponential decay. Therefore, discussions have traditionally been based on the rate equations for spin states. On the other hand, it is theoretically predicted that spin dynamics exhibit a characteristic known as coherent quantum beats, a phenomenon that has been observed in the delayed fluorescence particularly in the field of radiation chemistry[1]. It is because spin dynamics exhibiting quantum beats contribute only to the gradient, i.e., decay coefficient of the radical pair or growth of the product monitored in TA signal. Furthermore, in long-lived radical pairs, decoherence causes the radical pair to enter a so-called pseudo-stationary state.

Despite theoretical speculation that coherent dynamics are likely important for low-field effects (LFEs), there are few examples of quantitative observations of the relationship between spin dynamics and LFEs in the time domain. Considering the mechanisms of decoherence in spin systems, it cannot be ruled out that low-field effects exist even in pseudo-stationary states. In this study, we focused on this issue and experimentally investigated the relationship between methods for observing coherent spin dynamics and the low-field effect. To observe coherent spin dynamics in the time domain, we used a complementary approach combining the pump-push spectroscopy method established by Lambert et al. [2] with nanosecond-scale magnetic field switching.[3, 4]

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Invited Lecture

Magnetically Enhanced Photocurrent in Organic Photovoltaic Materials Due to Spin-polarized Triplet States

Tomoaki Miura[1]

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The recent emergence of non-fullerene acceptors such as Y6 has driven organic thin-film solar cell efficiencies toward ~20%, largely attributed to near-unity exciton dissociation and high carrier mobilities.[1] The latter advance, however, appeared to preclude meaningful magnetic field effects (MFEs) due to the resulting ultrashort radical-pair lifetimes — a prospect discouraging for spin chemists.

To investigate spin and carrier dynamics in organic photovoltaic (OPV) films, we developed simultaneous optical and electrical detection (SOED), a methodology that independently and quantitatively resolves time-dependent photocarrier concentration and mobility. Initial studies on the classical P3HT:$PC_{61}BM$ blend confirmed negligibly small MFEs on photocurrent at room temperature, seemingly validating pessimism about MFEs in modern OPV systems.[2]

Contrary to these expectations, we observed positive MFEs of a few % on both photocurrent and transient absorption signals in PTB7:$PC_{71}BM$ films at room temperature (MFEs on the carrier concentration, Fig. 1). The broad MARY spectra and very fast rise of MFE (< 10 ns) rule out the conventional radical-pair mechanism. Through systematic variation of excitation intensity and temperature, together with comparison against neat PTB7 films, we identified that the observed MFE is due to a novel triplet mechanism, involving spin-polarized triplet excitons undergoing sublevel-selective deactivation. Consequently, triplet-channel carrier generation pathway is demonstrated in the modern OPV material, which is contrary to the widely accepted popular belief that charge separation occurs solely from the singlet exciton.

Analogous MFEs on photocurrent were subsequently observed in PM6:Y6 films — the current state-of-the-art OPV system. These findings demonstrate the possibility of magnetically enhanced photovoltaic conversion efficiency based on the triplet mechanism. Mechanistic details will be presented.

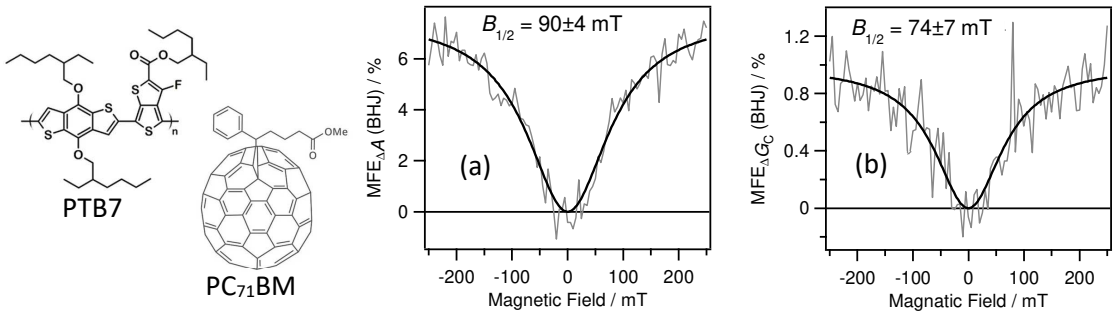

Fig. 1 MFEs on the transient absorption (a) and transient photocurrent (b) signals of the PTB7:$PC_{71}BM$ film at 10 ns at room temperature.

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Contributed Lecture

Spin-Selective Photochemistry: Magnetic Control of Singlet Oxygen through Upstream Radical Pair Dynamics

Yeongcheol Ki[1], Seungmin Choi[1], Dongcheol Park[1], Yeri Son[1], Hyun Gu Kang[1], Hyeongyeol Oh[1], Won-jin Chung[1], Lewis M. Antill[2*], Hohjai Lee[1*]

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[2]Korea Biomedical Institute for Global Health Research and Technology (K-BIGHEART), Pohang University of Science and Technology (POSTECH), Pohang 37673, Republic of Korea

Singlet oxygen, $O_2(^1\Delta g)$, is a key reactive intermediate in photodynamic therapy, photocatalysis, and oxidative chemistry, yet its generation through conventional triplet sensitization is inherently insensitive to external magnetic fields. We report that singlet oxygen generation can be magnetically tuned by embedding a spin-correlated radical pair as an upstream control element, decoupled from the downstream oxygen activation step. Using a covalently linked pyrene-dimethylaniline (Py-DMA) donor-acceptor system in aerated acetonitrile, we demonstrate that hyperfine-driven singlet-triplet interconversion within the photogenerated radical pair selectively gates the triplet channel that leads to singlet oxygen formation, while molecular oxygen itself does not participate in the spin-sensitive step.

Two complementary optical observables, exciplex fluorescence and $O_2(^1\Delta_g)$ near-infrared phosphorescence, serve as simultaneous reporters of the singlet- and triplet-derived reaction pathways, respectively. Both signals respond to an applied magnetic field with opposite signs yet share an identical half-saturation field value of $B_{1/2} \approx 18.4$ mT, providing direct spectroscopic evidence for their common spin origin. Time-resolved measurements further establish that the magnetic field modulates $O_2(^1\Delta_g)$ yield without affecting its excited-state lifetime, confirming that spin dynamics act strictly upstream of the oxygen activation chemistry. Semiclassical spin-dynamics simulations quantitatively reproduce both the field dependence and the opposing MFE signs of the two signals.

These results establish a general design principle for spin-chemical control of photochemical reactivity, in which a radical pair functions as a modular magnetic-field-sensing element structurally and mechanistically separable from the downstream chemistry it governs. The implications for magnetically switchable photosensitizers and field-responsive reactive oxygen species generation will be discussed.[1]

[1] 'Upstream Spin Control of Singlet Oxygen Generation through Radical Pair Dynamics', Y. Ki, S. Choi, D. Park, Y. Son, H. G. Kang, H. Oh, W.-j. Chung, L. M. Antill, and H. Lee, *submitted*.

Contributed Lecture

Optically detected and radio wave-controlled spin chemistry in flavoproteins

Kun Meng[1,2], Linyan Nie[1,2], Johannes Berger[3], Nick R. von Grafenstein[1,2], Christopher Einholz[1,2,3], Stefan Weber[3], Lars-Oliver Essen[4], Roberto Rizzato[1,2], Erik Schleicher[3], Dominik B. Bucher[1,2]

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[2] Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799, München, Germany
[3] Albert Ludwigs-Universität Freiburg, Institute of Physical Chemistry, 79104 Freiburg, Germany
[4] Marburg University, Chemistry Department, 35032 Marburg, Germany

Optically addressable spin systems are a cornerstone of quantum sensing; however, established platforms, primarily solid-state defects, offer limited (bio)chemical tunability. Here, we introduce flavoproteins as a new class of optically readable and radio-frequency (RF) controllable spin systems that operate under ambient conditions. We demonstrate optically detected magnetic resonance (ODMR) in the photoactive proteins cryptochrome and improved light–oxygen–voltage (iLOV) domains, originating from spin-correlated radical pairs generated upon blue-light excitation and their associated spin chemistry. By applying RF fields, we manipulate the radical pair spin chemistry and read out its dynamics via changes in flavin fluorescence. The resulting ODMR signals exhibit high contrast, reaching up to ~50% in iLOV.

In the talk, we will discuss the first applications of these systems. ODMR enables magnetic field imaging using a fluorescence microscope, providing a route toward genetically encodable quantum sensors. Furthermore, the combination of magnetic field gradients and RF excitation allows spatially selective control of spin chemistry, which can be directly visualized via fluorescence.

In the final part of the talk, we will give an outlook on potential applications ranging from bioimaging to genetically encoded quantum sensors and RF-controlled spin chemistry for biochemical control.

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Contributed Lecture

Modifying the photochemistry in flavoproteins

Christopher Einholz[1,2], Johannes Berger[1], Johannes Ruhnke[1], Anton Schmidt[1], Philipp Seckinger[1], Stefan Weber[1], Erik Schleicher[1]

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Flavocoenzymes are nearly ubiquitous in the catalysis and regulation of a wide array of biological processes [1]. However, the functional potential of these proteins is limited by the availability of canonical amino acids and standard flavin cofactors. The use of chemically modified protein building blocks allows for the development of proteins with optimized properties, ranging from altered reactivity to increased stability. Leveraging novel in vivo systems, we are now able to incorporate both modified flavins and non-natural amino acids into any flavoprotein.

These altered properties were evaluated using two established systems: (i) cryptochromes, which undergo long-distance light-induced electron transfer [2], and (ii) LOV domains, which induce signal transduction through light-driven covalent bond formation. Using time-resolved spectroscopy, we observed significant changes in the photochemistry and recombination kinetics of various cryptochrome and LOV proteins. Notably, we modulated the magnetic sensitivity of cryptochromes through modifications of the electron transfer chain and, for the first time, via chemical modification of the FAD cofactor [3], while also achieving considerable improvements in the fluorescence properties of LOV domains.

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Invited Lecture

Singlet Exciton Fission and Triplet Triplet Annihilation Studied with Transient Magneto Optical Spectroscopy

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Singlet fission (SF) and triplet-triplet annihilation (TTA) are fascinating exciton interconversion processes with the potential to significantly boost solar cell efficiency. SF converts a high-energy singlet exciton into two lower-energy triplet excitons, while TTA performs the inverse, combining two triplets into one emissive singlet. For solar energy applications, harnessing these long-lived triplet states allows photovoltaics to overcome conventional thermalisation losses[1], generate up-converted light[2], or enhance carotenoid-to-bacteriochlorophyll energy transfer in photosynthetic light-harvesting complexes[3].

Crucial to controlling these pathways is understanding the multi-exciton intermediate states involved. While the formation of a spin-2 quintet state often acts as a loss mechanism in photovoltaic systems, for example, it simultaneously presents an exciting opportunity for quantum technologies due to its potential for room-temperature electronic spin coherence[4,5].

In this talk, I will describe recent work from my group on characterising the dynamics of SF and TTA across a range of molecular and biological systems. I will discuss how we use ultrafast time-resolved optical and transient magneto-optical spectroscopy to untangle these complex spin states and map their trajectories.

[1] Nagaya et al., Exciton Fission Enhanced Silicon Solar Cell, *Joule*, 9, 101965 (2025). https://doi.org/10.1016/j.joule.2025.101965

[2] Polak, et al. "Manipulating molecules with strong coupling: harvesting triplet excitons in organic exciton microcavities."*Chemical Science* 11, 343-354 (2020).
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[3] Wang, *et al.* "Singlet fission contributes to solar energy harvesting in photosynthesis." *arXiv preprint arXiv:2411.18801* (2026).
https://arxiv.org/abs/2411.18801

[4] Ishii, *et al.* "Macrocyclic parallel dimer showing quantum coherence of quintet multiexcitons at room temperature."*JACS* 146.37 (2024): 25527-25535.
https://doi.org/10.1021/jacs.4c05677

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https://chemrxiv.org/doi/full/10.26434/chemrxiv.15001885/v1

Invited Lecture

Optical Readout of Molecular High-Spin States at Room Temperature

Jeannine Grüne[1]

[1]*Department of Materials, University of Oxford, UK*

High-spin states are crucial in various organic applications, spanning from optoelectronics to quantum technologies. Despite significant progress in generating spin-polarised high-spin states, their optical detection under ambient conditions remains a major challenge for the development of practical spin-based technologies.

This talk will discuss the generation, characterisation, and optical readout of molecular high-spin states using complementary magnetic resonance techniques, including transient electron paramagnetic resonance (trEPR) and optically detected magnetic resonance (ODMR). Particular emphasis will be placed on strongly spin-polarised triplet and quintet states produced by singlet fission, which offer access to molecular spin systems with multiple addressable spin sublevels. Our recent studies demonstrate how molecular structure governs high-spin state formation as well as their participation in emissive pathways and optical readout up to room temperature, enabling direct molecular interfaces between high-spin states and light. [1]

Building on these developments, zero-field ODMR provides access to molecular spin states under conditions relevant for practical operation. Optical spin readout, the connection between spin states and luminescence, and the role of different molecular high-spin multiplicities will be discussed in the context of room-temperature operation and the absence of external magnetic fields. These developments open new opportunities for studying and controlling spin-dependent processes in organic materials under ambient conditions.

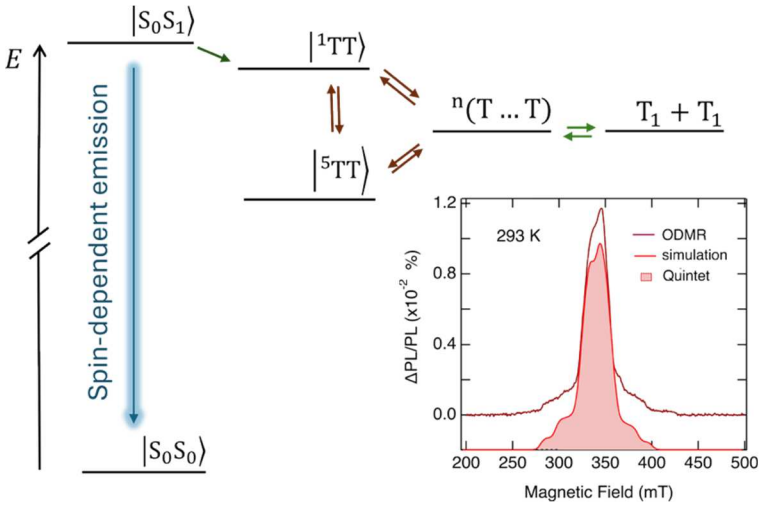

Fig. 1. High-spin state dynamics in intramolecular singlet fission, including quintet-mediated emission up to room temperature.

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

Contributed Lecture

Room temperature optical read-out of triplet states in (6,5) SWCNTs

J. Alejandro de Sousa[1]*, Ilias Vandevenne[1], Jana Nikolić[1], Tuur Boonen[1], Etienne Goovaerts[1], Sofie Cambré[1]

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Optically addressable triplet states are one of the most promising systems for being implemented as quantum sensors. The possibility of initializing and reading spin polarizations using optical photons instead of microwave photons offers high sensitivity. Triplet states allocated in NV^- centers have already been exploited for ultrasensitive detection of small magnetic fields, electrical currents, temperature, and analyte concentrations with high precision.[1] In the search of new systems for quantum sensing, single-walled carbon nanotubes (SWCNTs) emerge as a promising platform due to the possibility of tuning their strongly-bound excitonic states even at room temperature via internal and external functionalization, biocompatibility, emission in the skin transparency and optical data communication range (1000-1400 nm).[2] To experimentally resolve the characteristics of triplet states, we implement the optically detected magnetic resonance (ODMR) technique.[3,4] This allows for monitoring the transitions between triplet sublevels in an externally applied magnetic field through the emission from the sample, combining the sensitivity of emission spectroscopy with the spin sensitivity of magnetic resonance. However, even when singlet excitons have been extensively studied on SWCNTs, triplet-state properties remain largely unknown, and even more for sp^3 functionalized SWCNTs. In previous studies, we decorated SWCNTs with sp^3 defects and our experimental and theoretical calculations confirm the localization of the triplet excitons around the defect.[5] Here, we demonstrate for the first time that chemically induced sp^3 defects with aryl moieties lead to an enhanced ODMR contrast, permitting optical addressability at room temperature.[6] Additionally, new ODMR features evolve with increasing temperature, pointing to a change in the exciton dynamics when the external magnetic field is aligned with the main nanotube axis. Simultaneous fitting of the ODMR spectra was performed using the Easyspin platform by combining two excitons with different zero-field splitting parameters. Finally, we demonstrate for the first time the sensitivity of the triplet states allocated in SWCNTs towards a specific chosen paramagnetic analyte. Furthermore, we achieve on-chip addressability, opening new opportunities for point-of-care sensors. These findings highlight how the functionalization of SWCNTs with sp^3 defects offers a powerful strategy to control TE dynamics for implementation in quantum sensing applications.

[1] T. F. Segawa et al., Prog. Nucl. Magn. Reson. Spectrosc. **2023**,134-135, 20-38.
[2] J. Zaumseil et al., Adv. Opt. Mater. **2022**, 10, 2101576.
[3] E. Goovaerts, eMagRes, **2017**, 343.
[4] I. Sudakov et al., ACS Nano, **2023**, 17, 2190.
[5] J. A. de Sousa et al., ACS Nano, **2025**, 19, 36384.
[6] J. A. de Sousa et al., Submitted, **2026**.

Flash Talks

Flash Talk

A tale of light and shadow: Room-temperature magnetoluminescence in asymmetric organic biradicals

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Asymmetric organic biradicals provide a molecular route to tune optical emission with spin dynamics, particularly when a 'dark' radical perturbs the photophysics of its luminescent radical partner. TEMPO-Pho-TTM has recently demonstrated this bright-dark biradical concept, exhibiting magnetophotoluminescence attributed to hyperfine coupling, Δg-mediated spin mixing and spin polarization between the nitroxide and trityl radical centres [1]. Here, we further the study by functionalising the TTM unit with a series of carbazole-substituted bright radical derivatives, introducing donor-to-TTM charge transfer character into the emissive radical centre. This molecular series allows us to test whether increased push-pull character enhances optical brightness while preserving the hyperfine-sensitive spin branching. Room-temperature magneto steady-state and transient photoluminescence are used to distinguish changes in photoluminescence quantum efficiency from changes in spin-dependent branching and decay. This work aims to define design rules for increasing magnetosensitivity at room-temperature by balancing radiative rate, charge-transfer character and spin communication in bright-dark biradicals.

[1] Wang, Xing, et al. "Spin-Correlated Luminescence Enabled by Bright–Dark Radical Pairing in a Diradical System." *Angewandte Chemie* 137.40 (2025): e202513593.

Flash Talk

Magnetic field effects of radical-exciplex systems

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[2]*Department of Chemistry, University of Rennes, Rennes, France*

The electron spin nature of excited states underpins charge transfer and recombination processes in the photochemistry of materials towards a range of applications including organic light emitting diodes (OLEDs), photovoltaics and sensors. Magnetic field effects (MFEs) have been used to probe the interplay between excited state complexes (exciplexes) and spin-correlated radical-ion pairs where hyperfine-driven singlet-triplet spin mixing provides the basis for magnetic-field sensitive photophysics.
Here we investigate the magnetosensitivity of exciplex model systems (e.g. dimethyl-anthracene/dimethyl-aniline, phthalimide/carbazole) with potential for MFE read-out from fluorophore and exciplex components [1, 2]. Tunable sensitivity of the relative sign and magnitude of the MFEs with ratiometric response from dual-emission properties of the system are explored. We consider how the introduction of stable organic radicals (trityl, nitroxide) modulates the field-response of exciplex system by additional redox reactions and enables new magneto-optical behaviour from radical-coupling singlet-tri-plet states to doublet-quartet manifolds [3].

[1] S. Richert, A. Rosspeintner, S. Landgraf, G. Grampp, E. Vauthey, D. R. Kattnig, Time-Resolved Magnetic Field Effects Distinguish Loose Ion Pairs from Exciplexes, *J. Am. Chem. Soc.*, 2013, **135**, 15144–15152.
[2] P. Sumsalee, P. Morgante, G. Pieters, J. Crassous, J. Autschbach, L. Favereau, Nega-tive Solvatochromism and Sign Inversion of Circularly Polarized Luminescence in Chiral Exciplexes as a Function of Solvent Polarity, *J. Mater. Chem. C*, 2023, **11**, 8514–8523.
[3] Y. Mori, Y. Sakaguchi, H. Hayashi, Magnetic Field Effects on Chemical Reactions of Biradical Ion Pairs in Homogeneous Fluid Solvents, *J. Phys. Chem. A*, 2000, **104**, 21, 4896-4905

Flash Talk

Elucidation of spin-correlated emission of a carbazole-containing diradical emitter

Asato Mizuno[1,2,3], Ryota Matsuoka[1], Shojiro Kimura[4], Tetsuro Kusamoto[1,2,3,5]

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[2]*OTRI-Spin, The Univ. of Osaka, Japan*
[3]*CSRN, The Univ. of Osaka, Japan*
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Luminescent radicals have been widely studied as a new class of molecular systems exhibiting novel photofunctions derived from their open-shell electronic structures.[1] Recent studies on luminescent triarylmethyl diradicals have shown intriguing spin-dependent emission (i.e., spin-correlated emission), as exemplified by magnetic-field effect on luminescence (i.e., magnetoluminescence).[2] Such luminescent diradical systems serve as simple model systems for understanding spin-correlated emission of radicals, but their variety remains limited. Especially, the correlation between larger intramolecular exchange interactions ($|2J/k_B|$ > ca. 10 K) and luminescence properties in diradicals has not been elucidated in detail.

Herein, we synthesized a novel carbazole-containing diradical emitter **1** (Fig. 1a) and investigated its emission properties at various temperatures and magnetic fields.[3] ESR measurements of **1** in frozen toluene estimated a $2J/k_B$ value of −24 K. Diradical **1** dispersed in a poly(methyl methacrylate) (PMMA) (0.01 wt%, **1_PMMA_0.01**) exhibited magnetoluminescence as well as thermally activated emission at cryogenic temperatures (Fig. 1b,c). These luminescence properties were distinctly different from those of the corresponding monoradical **2**. Detailed luminescence measurements under high magnetic fields revealed that the spin-correlated emission of **1** is explained by changes in spin populations in the electronic ground states. In this presentation, we will discuss the luminescence properties of **1**, in comparison with those of **2**.

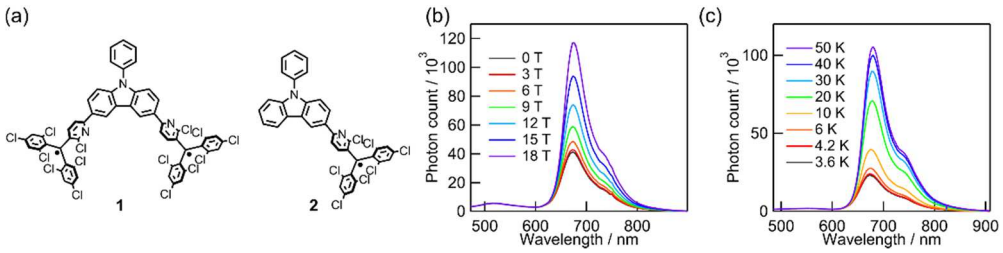

Figure 1. Chemical structures of carbazole-containing luminescent radicals **1** and **2**. (b) Magnetic-field dependence of the emission spectra of **1_PMMA_0.01** at 4.2 K (λ_{ex} = 375 nm). (c) Temperature dependence of the emission spectra of **1_PMMA_0.01** in the absence of a magnetic field (λ_{ex} = 375 nm).

[1] A. Mizuno, R. Matsuoka, T. Mibu, T. Kusamoto, *Chem. Rev.* **2024**, *124*, 1034.
[2] R. Matsuoka, S. Kimura, T. Miura, T. Ikoma, T. Kusamoto, *J. Am. Chem. Soc.* **2023**, *145*, 13615.
[3] A. Mizuno, R. Matsuoka, S. Kimura, K. Ochiai, T. Kusamoto, *J. Am. Chem. Soc.* **2024**, *146*, 18470.

Flash Talk

Host-guest Crystal Engineering Tailors the Room Temperature Spin Dynamics in Molecular Quantum Materials

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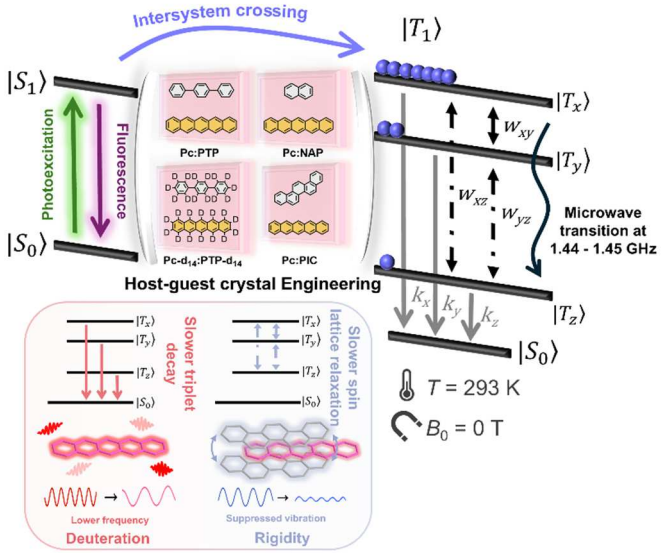
[1]*Department of Materials and London Centre for Nanotechnology, Imperial College London, Prince Consort Road, London, SW7 2AZ, UK*
[2]*Advanced Research Centre, James Watt School of Engineering, University of Glasgow, Glasgow, G11 6EW, UK*
[3]*Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA*
**Corresponding authors*

Molecular materials that retain electron spin coherence at room temperature are promising candidates for quantum technologies, including masers [1], that offer ultra low-noise microwave amplification and sensing. In particular, host–guest molecular crystals enable independent control of spin-active guests and their local environments to provide a tuning handle on spin-dependent device performance. Using a combined approach with electron paramagnetic resonance and optically-detected magnetic resonance [2], we systematically investigate the host-dependent spin dynamics of photoexcited pentacene triplet states doped into a series of molecular crystals: naphthalene, picene, *para*-terphenyl and perdeuterated *para*-terphenyl with perdeuterated pentacene. We reveal that by host modulation of the lattice rigidity and vibrational coupling controls triplet (de)population, spin relaxation and decoherence. Importantly, as the most rigid host, picene, significantly slows spin–lattice relaxation at the cost of reducing triplet spin polarisation, whilst deuteration reduces both the hyperfine-mediated inhomogeneous linewidth and vibrationally-mediated triplet depopulation. Consequently, the optical maser threshold and cooperativity are significantly improved for perdeuterated pentacene in perdeuterated *para*-terphenyl, which is also found to be the most viable candidate for building a continuous wave (cw) maser. This work demonstrates crystal engineering as an important and practical method for tuning the spin-dependent performance of quantum technologies.



[1] M. Oxborrow, J. D. Breeze and N. M. Alford, *Nature*, 2012, **488**, 353–356.
[2] S. K. Mann, A. Cowley-Semple, E. Bryan, Z. Huang, S. Heutz, M. Attwood and S. L. Bayliss, *Journal of the American Chemical Society*, 2025, **147**, 22911–22918

Flash Talk

Perylene Diimide(PDI) Based Chromophore-Radical Architectures for Long-Lived Photoexcited Spin States and as Promising Molecular Qubit Candidates

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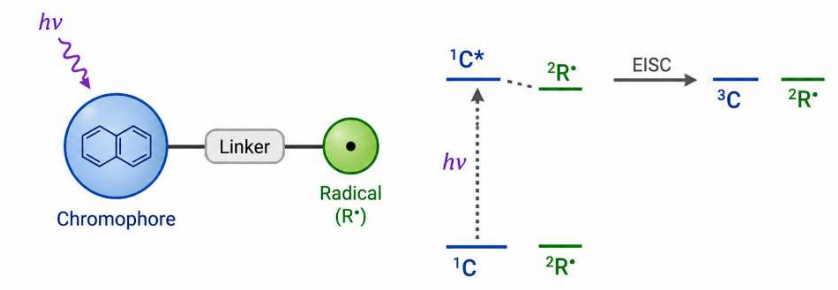
Photoexcited chromophore-radical systems are promising molecular platforms for quantum information science owing to their chemical tunability and ability to generate well initialized spin-sates through optical excitation [1].In particular, the combination of long-lived triplet-doublet states and controllable exchange coupling offers promising opportunities for molecular qubits and multilevel quantum systems. Perylene Diimide (PDI) is a particularly attractive chromophore due to its exceptional photostability, strong visible-light absorption, and favorable excited-state properties.



Here, we investigate photoexcited PDI-based chromophore-radical systems with the goal of understanding how the nature of the radical influences the photophysical and spin properties of the resulting assemblies. Particular emphasis is placed on the relationship between molecular structure and key parameters such as the excited-state's lifetime and stability, coherence time, and spin-spin coupling magnitude between the chromophore and radical components. Previous studies have shown that the spin properties of chromophore-radical systems are governed by exchange and dipolar interactions between the chromophore triplet state and the radical spin center, while the choice of chromophore, radical, and linker can strongly influence the resulting coupling regime and spin dynamics [1]. We identify the factors governing the development of photoactive molecular systems capable of controllable spin manipulation for quantum information science applications [1,2].

[1] Quintes, T.; Mayländer, M.; Richert, S. Properties and applications of photoexcited chromophore-radical systems. *Nat. Rev. Chem.* **2023**, *7*, 75-90

[2] Mayländer, M.; Kopp, K.; Hett, T.; Schwering-Sohnrey, M. F.; Richert, S.; Schiemann, O. PDI-trityl dyads as photogenerated molecular spin qubit candidates. *Chem. Sci.* **2023**, *14*, 10727-10735.

Flash Talk

Simple 3d-metal complexes for Magnetic Refrigeration

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This project entails synthesizing molecular materials with large magnetocaloric effects, as these materials could be suitable for magnetic refrigerators at liquid helium temperatures, based on adiabatic demagnetization. As helium is a non-renewable but fundamentally important cryogen, developing new cryogenic materials are of great societal importance. In this project the series of $A(NH_3)_6BF_6$ (A: Co, Cr ; B: V, Cr, Mn, Fe, Co, Ga) and $Co(NH_3)_6VOF_5$ and $Cr(NH_3)_6VOF_5$ have been crystalized, [1]. All samples crystalize in the cubic Pa3- space group. The unexplored magnetocaloric effect of these have been calculated from the magnetization of the samples, where $Cr(NH_3)_6FeF_6$ has the largest MCE (see Figure 1). The stability of the fluoride complexes enhances the possibility of commercial usage. The site symmetry of the metal centre MF_6^{3-} is not cubic but slightly distorted, with a C_3 axis as the highest symmetry axis, which is taken as the principal axis. For determination of the zero-field splitting of $Cr(NH3)_6^{3+}$, CrF_6^{3-}, MnF_6^{3-} (both perpendicular and parallel mode has been measured), FeF_6^{3-}, and VOF_5^{3-} CW-X-band EPR has been measured for all systems doped in $Co(NH_3)_6GaF_6$. For the axial system we add in both a, D, and F parameters. We have fitted the spectrum with a, D, F and all together. The zero-field splitting is very small, and it is difficult to get the information. Thus, high field EPR remains to be measured in Grenoble, along with the heat capacity of the entire series in Zaragoza.

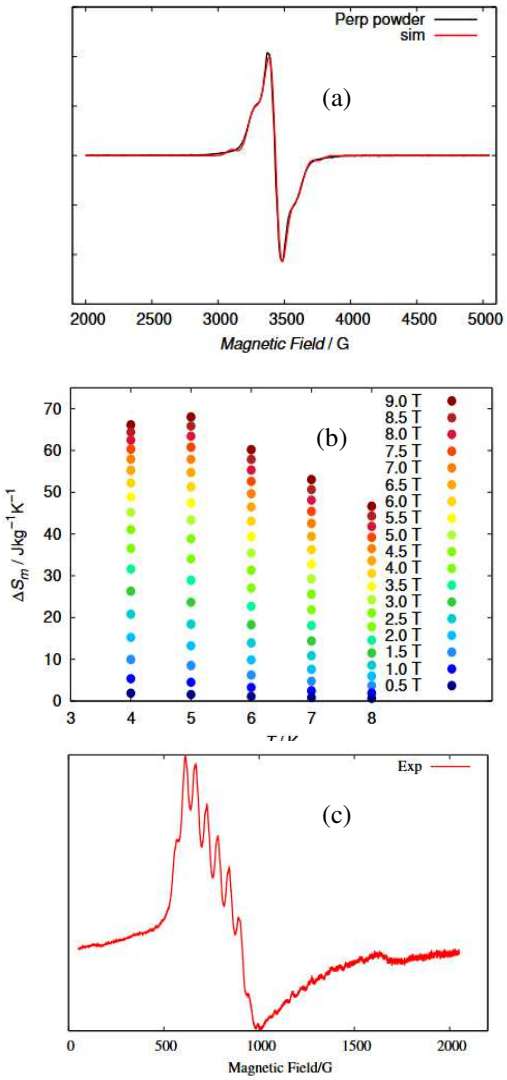

Figure 1. (a) RT CW-X band perpendicular mode EPR of FeF_6^{3-} 1% in $Co(NH_3)_6GaF_6$
(b) calculated MCE from the magnetization of $Cr(NH_3)_6FeF_6$ ([2])
(c) RT CW-X band parallel mode EPR of MnF_6^{3-} 1% in $Co(NH_3)_6GaF_6$

[1] Karl Wieghardt K., Siebert H. *Journal of Molecular Structure*, 1971, 7(3-4)
[2] Evangalisti M., Brechin E. K., *Dalton Trans., 2010, 39,* 4672-4676

Flash Talk

Electrically Detected Magnetic Resonance Characterisation of Donors in Silicon

M. M. Solly[1], N. F. L. Collins[1,2], J. Jacobs[1], A. Alsulami[2], F. Tuna[1,3], D. N. Jamieson[2], R. J. Curry[1]

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[2]*School of Physics, University of Melbourne, Parkville, Melbourne, VIC 3010, Australia.*
[3]*Department of Chemistry, University of Manchester, M13 9PL*

Donor spins in silicon have a promising role in the development of semiconductor-based quantum computers. Traditionally, the readout of the spin signal has been performed using electron paramagnetic resonance (EPR). However, the sensitivity of EPR is limited to approximately f 10^{10} spins for semiconductors, which limits the study of systems with fewer spins [1]. Electrically detected magnetic resonance (EDMR) technique is considered more advantageous for the study of spins in semiconductors since the magnetic resonance is detected via change in the conductivity of the sample and therefore is very sensitive to centers influencing the conductivity of the sample [2]. Here we use continuous wave EDMR (CW-EDMR) to characterise the spins of group V donors implanted in silicon (Si). We record the current change that results from a RF induced spin flip of either the electron localised on the donor ion, or the electron at the P_{b0} center found at the Si-SiO_2 interface. This modulates the population of photoexcited carriers in a spin dependent recombination process. The device includes an implanted region, a surface coplanar waveguide for RF delivery to the active region, a heavily doped source and drain electrode for electrical readout and a ground plane. We study the spin signal from ^{31}P, ^{75}As, and P_{b0} at the low RF frequency regime (20MHz-800MHz) corresponding to a magnetic field of 0 - 40mT, at 10K using a 405nm laser for optical excitation. The EDMR spectra from the device are shown in Fig: 1 with the peaks from ^{31}P and ^{75}As ions, and Pb_0 fitted to their transition positions according to theory.

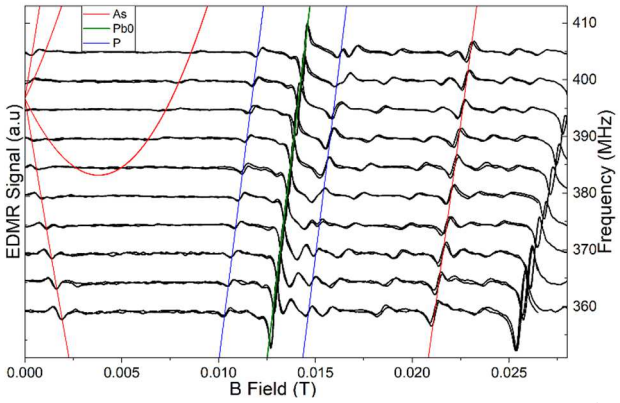

Figure 1: EDMR spectra of the device showing the transition peaks of ^{31}P, ^{75}As, and P_{b0}

[1] McCamey, D. R., et al. "Electrically detected magnetic resonance in ion-implanted Si: P nanostructures." *Applied Physics Letters* 89.18 (2006).

[2] Boehme, Christoph, and Klaus Lips. "The ultra-sensitive electrical detection of spin-Rabi oscillation at paramagnetic defects." *Physica B: Condensed Matter* 376 (2006): 930-935.

Flash Talk

Using spin as a probe to understand charge recombination in organic solar cells: an EDMR study

Lorenzo Catini[1], Jack Ovens[1], Luke Hanley[1], Claudia Tait[1]

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Organic Solar Cells (OSCs) possess unique properties such as tuneability and flexibility but are still inferior to other commercial solar energy technologies in terms of efficiency. This limitation mainly arises from the recombination of photogenerated charges on donor and acceptor molecules. Pulse Electrically Detected Magnetic Resonance (pEDMR) spectroscopy can provide unique insights into solar cells under operation by coherently manipulating spins directly involved in current generation and measuring the subsequent microwave-induced change in current arising from spin-dependent electronic transitions [1]. By exploiting spin as a probe, pEDMR can therefore be used to identify charged states involved in recombination and gain an improved mechanistic understanding of this process, informing guidelines for future molecular design aimed at developing more efficient devices.

In this work, a thorough characterisation of the spectral signatures of charged states involved in current generation was achieved for a range of donor:acceptor blends by investigating the magnetic field dependence of the pEDMR response. The role of these charged states in spin-dependent processes was then identified using Rabi nutation experiments, which highlighted two different mechanisms acting as loss pathways. The observation of spin-locking revealed bipolar recombination between a pair of coupled donor and acceptor spins, which was further confirmed by double-resonance experiments selectively addressing the acceptor spin and monitoring the response through the coupled donor spin [2]. The Rabi nutation experiment also uncovered a second mechanism involving the interaction between a triplet state and charged states, resulting in triplet annihilation and current quenching. Overall, this comprehensive investigation of different donor:acceptor blends uncovered crucial information on major loss pathways in organic solar cells.

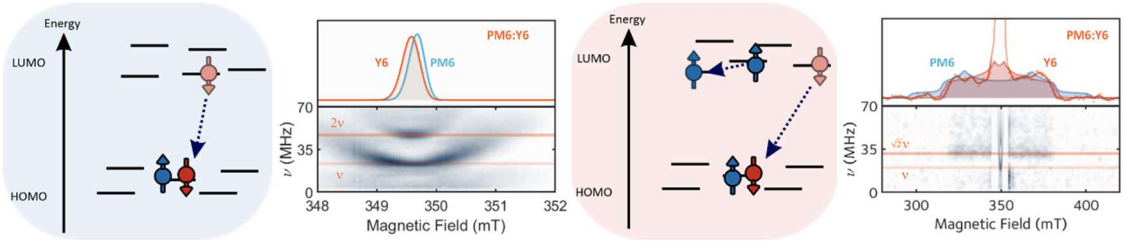


Figure 1. Schematic representation of the spin-dependent triplet charge annihilation (left) and bipolar recombination mechanisms (right) accompanied with experimental data supporting the assignment.

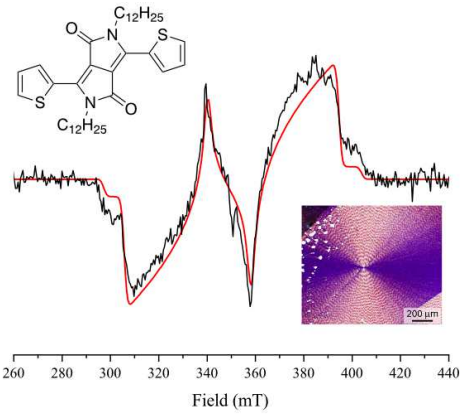
[1] C. Boehme et al., *eMagRes*, 6, 83-100, **2017**.
[2] A. J. Kupijai et al., *Phys. Rev. B*, 92, 245203, **2015**.

Flash Talk

Triplet Pathways in Twisted Crystalline Diketopyrrolepyrrole Films

Trent McHenry[1], Antti-Pekka Reponen [2], Tejas Deshpande [3], Damon Michael de Clercq[3], Ilya Dergachev[1], Joseph Prentice[4], St. John Whittaker[1], Stephanie Lee[1], Claudia E. Avalos[1], Sascha Feldmann[3]

[1] *Department of Chemistry, New York University, New York, NY, USA*
[2] *Rowland Institute, Harvard University, Cambridge, MA, USA*
[3] *Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland*
[4] *Department of Materials, The University of Manchester, Manchester, UK*



Diketopyrrolopyrroles (DPP) are a family of stable, solution-processible organic semiconductors with characteristically strong absorption.[1] DPP has optoelectronic and organic photovoltaic applications, with chemical substitutions on the chromophore used to tune its photophysical characteristics. It has been demonstrated that via alteration of the substituted moieties, the triplet state can be accessed via a singlet fission process (SF),[2] spin-orbit intersystem crossing (SO-ISC),[3] and/or charge transfer mechanisms in molecular blends.[4] We perform fs- and ns-transient absorption (TA) measurements along with transient electron paramagnetic resonance (trEPR) of DPP-C12 films in twisted crystal films, standard films, and in variable concentration in a toluene glass. TA measurements are utilized to identify a process in DPP films with timescales of 47/69 ps, corresponding to the S_0S_1 -> ^{1}(TT) pathway, along with a long-lived triplet state. We observe triplets characteristic of an SO-ISC mechanism with trEPR ($P_x/P_y/P_z$ = 0.562: 0.056: 0.382) and no ^{5}(TT) or SF born triplet states. CASSCF-NEVPT2 calculations were done on models including a monomer, dimer (parallel and perpendicular) and trimer system to assess how the singlet and triplet energies and zero-field splitting parameters change across systems. An 8e8o active space gave D = -1899 MHz, E = 246 MHz, in decent agreement with experiment D= -1496 MHz and |E| = 331 MHz. Calculated spin orbit coupling constants of the dimer ranged from 0.10 to 0.75 cm^{-1} and near zero for the monomer suggesting a more efficient ISC process in the dimer.

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[3] Maity, N., et al. *Nat. Commun*, 2022, **13**, no. 1, 5244.
[4] Salvadori, E., et al. *JMCA*, 2017, **5**, no. 46, 24335-24343.

Flash Talk

Photoinduced spin interactions and dynamics in a copper(II)-free base porphyrin dimer

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Meso-meso linked metalloporphyrin-free base porphyrin dimers (MFP) are emerging as promising chromophore-qubit candidates and multilevel quantum systems (*qudits*). Photoexcitation of the organic chromophore and subsequent intersystem crossing enables the population of spin polarized quartet states.
Otpical spectroscopy, *ab initio* DFT calculations and Time-Resolved Electron Paramagnetic Resonance (TR-EPR) are employed, enabling the investigation of electron and nuclear spin polarizations alongside their temporal dynamics. The coupling of a Cu(II) porphyrin with the free-base porphyrin moiety results in enhanced intersystem crossing. The nature of the metal center affects the triplet-doublet exchange coupling and spin polarization. Hyperfine coupling with the Cu(II) metal ion results in nuclear spin polarization which is accompanied by selective population and depopulation of elextron spin sublevels.
These results demonstrate that photoexcitation of the organic chromophore provides a viable pathway for the initialization of electron and nuclear spin levels within *qudits* with applications in quantum information science and engineering.

Flash Talk

Room-temperature molecular quantum sensing of the Earth's magnetic field

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The carotenoid-porphyrin-fullerene (**CPF**) molecular triad is well-known among the spin chemistry community – the work by Maeda *et al*. demonstrated that photoexcitation of **CPF** generates a radical pair, which can respond to magnetic fields as low the Earth's magnetic field [1]. At that time interest in **CPF** was driven by the search for a proof-of-concept system for the radical pair based magnetoreception hypothesis. However, the burgeoning interest in molecular quantum information science served as motivation to revisit this molecule within the context of quantum sensing of magnetic fields [2].

However, so far **CPF** magneto-sensing behaviour has only been observed at cryogenic conditions as the field effect on the radical pair substantially diminish with increasing temperature elevated (all but disappearing at room temperature)- a deal-breaker for practical quantum sensing applications of **CPF**. Utilising broadband transient absorption spectroscopy we demonstrate that **CPF** field effects actually persist even at room temperature, but the species carrying the field sensitivity is a recombination triplet instead of the radical pair. Furthermore, spin dynamics simulations based on a semi-classical approximation to the Haberkorn equation [3] are used to uncover a complex interplay between non-Arrhenius electron transfer and the **CPF** radical pair field effects. Crucially, we demonstrate that highly sensitive cavity-enhanced spectroscopy **CPF** resolves the Earth's magnetic field event at ambient temperatures.

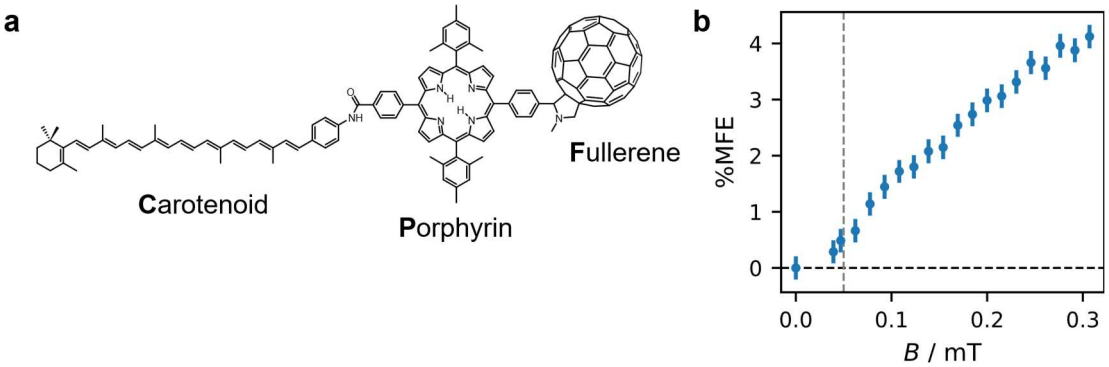

Figure: (a) Structure of **CPF** triad. (b) Sub-mT magnetic field effects on the yield of recombination triplet generated from CPF photoexcitation. Data has been recorded with an cavity-enhanced ringdown spectroscopy.

[1] Maeda K. et al. *Nature*, 453(7193):387–390, 2008.
[2] Tomoyasu M. *Chemical Physics Reviews*, 3(2):021301, May 2022.
[3] Alan M. L. et al. *The Journal of Chemical Physics*, 141(4):044111, 2014.

Flash Talk

Organic Carbenes as a Single Molecule Spin-Photon Interface

P. Mentzel,* S. Roggors, T. Unden, N. Striegler, A. Aubele, G. Bayer, O. Khavryuchenko, A. Salhov, J. Scharpf, M. B. Plenio, A. Retzker, F. Jelezko, T. R. Eichhorn, M. Pfender, P. Neumann, T. A. Schaub, I. Schwartz

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The development of scalable quantum technologies demands platforms that combine the robust coherence of solid-state spins with the precise tunability of atomic systems. While traditional inorganic lattice defects suffer from limited tunability, structurally tailored molecular platforms have emerged as highly customizable alternatives. In a previous study, we investigated a purely organic, ground-state triplet carbene in a host matrix, finding remarkable spin coherence as well as >40% optically detected magnetic resonance (ODMR) contrast in the ensemble measurements.[1]

To transition from bulk ensembles to discrete quantum control, we synthetically modified the molecular structure of both the carbene and the host matrix. This allowed us to achieve the first optical isolation and coherent control of an individual molecular spin-qubit. High-resolution confocal spectroscopy at 4.5 K reveals discrete, single-emitter close-to lifetime-limited zero-phonon lines, extended dynamical-decoupling coherence, prolonged spin relaxation times, and remarkable spectral stability.[2] By successfully bridging the gap between bulk behavior and single-molecule addressability, this work establishes bottom-up assembled molecular materials as a premier, scalable platform for single-emitter quantum optics.

[1] S. Roggors et al., *J. Am. Chem. Soc.*, **2025**, *147*, 36383-36392.
[2] S. Roggors et al., **2026**, *submitted.*

Flash Talk

Modular spin-optical interface in persistent molecular spin qubits

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Electron spins in molecules represent chemically tunable qubits for quantum sensing applications. In particular, optically addressable molecular spins offer attractive functionalities such as optical initialization and readout, enabling superior detection sensitivity and spatial resolution compared with microwave-based detection methods. In the context of external-field sensing, such as magnetic-field sensing, it is essential to tune the spin sublevel energies originating from spin–dipolar interactions for optimizing the trade-off between magnetic responsiveness and spin coherence time[1], yet it remains largely unexplored. Here, we elucidate the correlation between magnetic responsiveness and spin coherence time through the control of spin–dipolar interactions in chemically modulated fullerene spin qubits. Photoexcited triplet spin in fullerene exhibits relatively long T_2 due to less nuclear spins and small zero-field splitting (ZFS) parameters (D and E).

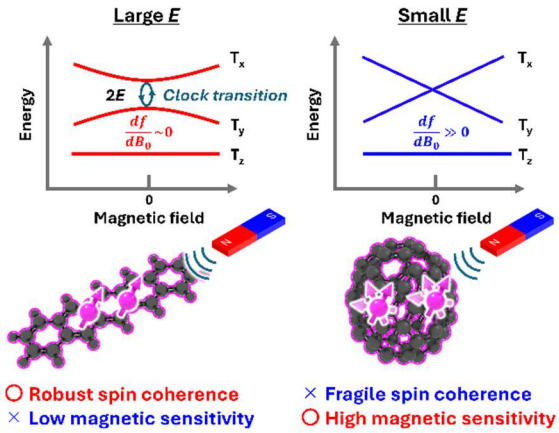

Figure 1. Trade-off between magnetic responsiveness and spin coherence time, depending on spin-dipolar interactions.

Substituted fullerenes (IC60BA, IC60TriA, IC70BA) were synthesized via Diels-Alder reactions. Transient absorption measurements revealed triplet lifetime on the microsecond timescale for the C60 derivatives and millisecond timescale for the C70 derivative in polystyrene films at room temperature. Transient EPR spectroscopy detected the photoexcited triplet spin manifolds with spin-lattice relaxation times of a few microseconds at room temperature. Zero-field optically detected magnetic resonance (ODMR) experiments at room temperature exhibited the signals corresponding to photoexcited triplet spins with the negative contrasts (<10^{-2} %). In contrast, the ODMR spectra at 77 K showed the opposite-sign signal with enhanced contrast (>10^{-2} %), suggesting suppression of spin-lattice relaxation due to reduced dynamic pseudo rotation of fullerene at lower temperatures. Furthermore, the spectral evolution as a function of magnetic field was found to depend strongly on the ZFS parameters, which could be controlled through chemical modification.

1. S. L. Bayliss *et al.*, *Phys. Rev. X.*, **2022**, *12* (3), 031028.

Flash Talk

Quantum sensing of time-dependent magnetic signals with molecular spins

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Quantum sensing has become an increasingly interesting application for spins, enabling tasks beyond the capabilities of classical counterparts [1]. Molecular spins can be embedded into superconducting resonators [2] for the detection of AC magnetic fields synchronized with the microwave (MW) sequence used to manipulate the spins themselves [3]. Further progress in this field can be made by extending the detection to non-periodic signals, as has been realized on NV centers [4]. To this end, we develop two sensing protocols based on the phase accumulation of electronic spins during an Hahn echo sequence, and we test them on two magnetically diluted molecular samples of VO(TPP) (S=1/2, I = 7/2) and of $VOPt(SOCPh)_4$ (S=1/2, I = 7/2) embedded in a superconducting YBCO (Fig. 1) [5]. A rafiofrequency (RF) coil is used to deliver the test signal, while manipulation, detection and signals generation are performed with the use of a home-made heterodyne system [3,5]. Tests are performed using different signals (e.g. Gaussian, square, double Gaussian) and the expected behaviour for the phase accumulation is experimentally confirmed. We report sensitivity of few $10^{-7}\ T/\sqrt{Hz}$, with lower bound approaching $10^{-8}\ T/\sqrt{Hz}$ [5].

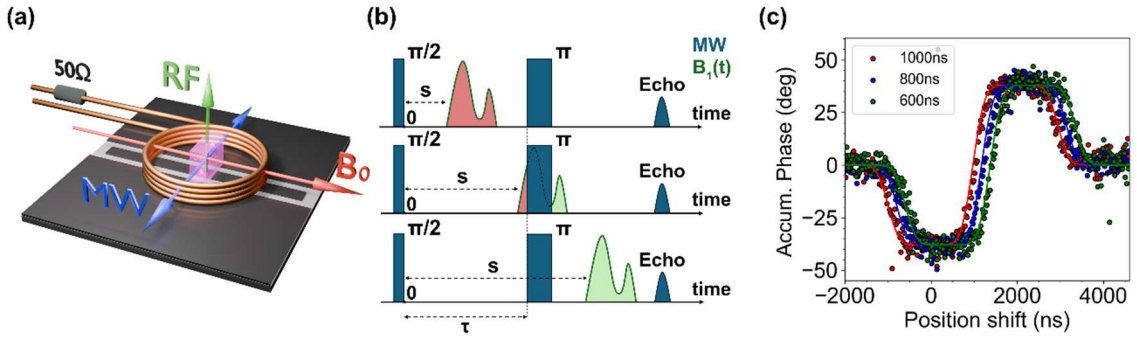

Figure 1 a) Experimental setup: YBCO coplanar resonator (black), spin sample (purple) and copper coil (orange). b) Scheme of one of the two protocols developed for sensing time-dependent magnetic fields. Each row indicates a successive step in the protocol execution. c) Resulting phase accumulation curves for a Gaussian signal: the starting position of the external signal is shifted resulting in a corresponding rigid shift in the phase accumulation curve.

[1] C.L. Degen, et al., *Rev. Mod. Phys*., **89**, 035002 (2017)
[2] F. Troiani, et al., *Journal of Magnetism and Magnetic Materials,* **491**, 165534 (2019)
[3] C. Bonizzoni, et al., *npj Quantum Inf., **10***, 41 *(2024)*
[4] J. Zopes, C.L. Degen, *Phys. Rev. Applied*, **12**, 054028 (2019)
[5] M. Lanza, et al., Phys. Rev. Applied **25**, 034045 (2026)

Flash Talk

Magneto-Optical Effects in Organic Radicals

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Magneto-optical activity from interactions of organic molecules with polarised light can be shown to originate from three mechanisms relating to their electronic structure.[1] They arise due to: degeneracy in excited states (A); mixing of excited states (B); and degeneracy in the ground state respectively (C). While several high-symmetry molecules have been shown to exhibit strong magneto-optical activity arising from the A-term, examples of paramagnetic materials which exhibit C-term behaviour are limited to transition metal and lanthanide complexes.[2]

Stable luminescent trityl radicals have been of significant interest in recent years due to their potential in efficient OLEDs and quantum sensors that operate using strong optical transitions between doubly-degenerate ground and excited states, $D_0 + h\nu \leftrightarrow D_1$.[3] Here we develop model systems based on mixtures of TTM-based radicals and triplet states of chromophores in solution, showing excited state and spin dynamics following photoexcitation that results in strong ground state spin polarisation at room temperature. Using a combination of Faraday rotation (magnetic circular birefringence) and magnetic circularly polarised luminescence, we explore organic radicals as magneto-optical materials via the spin-optical interface with polarised light.

[1] Z. Nelson, L. Delage-Laurin, and T. M. Swager, 'ABCs of Faraday Rotation in Organic Materials', *J Am Chem Soc*, vol. 144, no. 27, pp. 11912–11926, Jul. 2022, doi: 10.1021/jacs.2c01983.
[2] L. Delage-Laurin, H. K. S. Young, E. A. LaPierre, M. C. Warndorf, I. Manners, and T. M. Swager, 'C-Term Faraday Rotation in Low Symmetry tert-Butyl Substituted Polyferroceniums', *ACS Macro Lett*, vol. 12, no. 5, pp. 646–652, May 2023, doi: 10.1021/acsmacrolett.3c00032.
[3] M. R. Wasielewski *et al.*, 'Exploiting chemistry and molecular systems for quantum information science', *Nat. Rev. Chem.*, vol. 4, no. 9, pp. 490–504, Jul. 2020, doi: 10.1038/s41570-020-0200-5.

Flash Talk

Circularly polarized luminescence from a polybrominated triarylmethyl radical with a pyridyl ring

Taichi Hiramoto[1], Asato Mizuno[1,2,3], Wataru Ota[4,5], Tetsuri Takami[4,5], Emiko Fujiwara[4], Tohru Sato[4,5], Yuichi Kitagawa[6,7], Tetsuro Kusamoto[1,2,3,8]

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[2]OTRI-Spin, The Univ. of Osaka, Japan
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Luminescent radicals exhibit unique photophysical properties arising from their open-shell electronic structures[1]. In recent years, considerable attention has been paid to the circularly polarized luminescence (CPL) properties of the luminescent radicals. Triarylmethyl (TArM) radicals, which are representative luminescent radicals, can exhibit CPL owing to the chirality derived from their propeller-like structures. However, the racemization barriers of the TArM radicals are generally low, making optical resolution difficult[2]. As a result, reports on the CPL properties of the radicals are still limited. In this context, diversification of luminescent radicals with high racemization barrier is desired.

Herein, we designed and synthesized a novel luminescent chiral radical **1**, which is a brominated derivative of the reported TArM radical **2**[3] (Fig. 1a). The absorption and emission spectra of **1** were bathochromically shifted compared to those of **2** (Fig. 1b). Furthermore, thanks to the bromine substituents, optical resolution of **1** was successfully achieved, and the enantiomers exhibited mirror-image CPL spectra (Fig. 1c). In this presentation, we will discuss the effects of the bromine substitution on the luminescence and chiroptical properties of **1**.

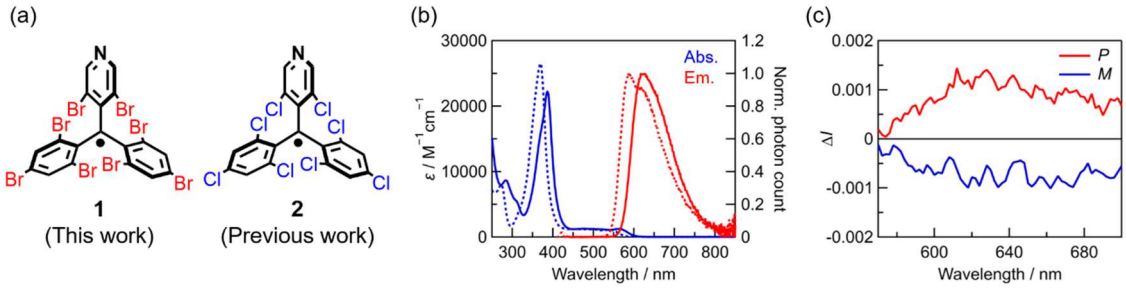

Fig. 1. (a) Chemical structures of 1 and 2. (b) Absorption (blue) and emission (red, l_{ex} = 450 nm) spectra of 1 (solid lines) and 2 (dashed lines) in CH_2Cl_2. (c) CPL spectra of P (red) and M (blue) enantiomers of 1 dispersed in a poly(methyl methacrylate) (PMMA) matrix (1 wt%, l_{ex} = 450 nm).

[1] A. Mizuno, *et al.*, *Chem. Rev.* **2024**, *124*, 1034.
[2] P. Mayorga-Burrezo, *et al.*, *Chem. Eur. J.* **2020**, *26*, 3776.
[3] Y. Hattori, *et al.*, *Angew. Chem. Int. Ed.* **2014**, *53*, 11845.

Flash Talk

Enhancements of Over a Factor 1000 by Rational Design of photo-Polarization Agents for Dye Sensitized Solid-state NMR

Máté Visegrádi,[1] Marcel Levien,[1] Ganesan Karthikeyan,[2] James W. Whipham,[1] Michael R. Wasielewski,[3] Olivier Ouari,[2] Federico De Biasi,[4] Lyndon Emsley[1]

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Nuclear Magnetic Resonance (NMR) spectroscopy is a versatile technique exploiting magnetic properties of spins of nuclei to obtain atomic level structural information. While NMR is a major analytical technique in the daily life of most synthetic chemists, certain applications are still challenging because of the low polarization of the nuclear spin-flip transitions.

Emerging pathways to generate bulk nuclear hyperpolarization in solids use optically based techniques such as photochemically induced dynamic nuclear polarization (photo-CIDNP).[1,2] Here, upon optical excitation of the system transient population differences between electronic states are exploited. Recently, we have shown that in solids it is possible to generate bulk hyperpolarization using small donor-acceptor molecules (D-A) as photo-polarizing agents (PAs).[2] Following the initial demonstration of ^{1}H bulk hyperpolarization at low magnetic field, we extended the approach to magnetic fields as high as 21.15 T with NMR signal enhancement factors reaching a factor of 100.[2]

To further guide the design of new photo-PAs we recently extended the existing kinetic photocycle description of the solid-state photo-CIDNP process, and here we show how this enables the rational design of a second generation of photo-PAs that reach unprecedentedly high ^{1}H enhancements at high magnetic fields, yielding ^{1}H enhancement factors over 1000. We will present experimental and theoretical results on the photo-CIDNP mechanisms that facilitate higher signal enhancements.[4,5]

[1] De Biasi, F.; Hope, M. A.; Avalos, C. E.; Karthikeyan, G.; Casano, G.; Mishra, A.; Badoni, S.; Stevanato, G.; Kubicki, D. J.; Milani, J.; et al. Optically Enhanced Solid-State 1H NMR Spectroscopy. *J. Am. Chem. Soc.* **2023**, *145* (27), 14874-14883.
[2] F. De Biasi, G. Karthikeyan, M. Visegrádi, M. Levien, M. A. Hope, P. J. Brown, M. R. Wasielewski, O. Ouari, L. Emsley *J. Am. Chem. Soc.* **2024**, *145*, 27, 14874–14883.
[3] F. De Biasi, M. Visegrádi, M. Levien, B. F. Chmelka, L. Emsley, *J. Chem. Phys*. **2025**, *163*, 244113.
[4] M. Levien, M. Visegrádi, G. Karthikeyan, G. Cassano, C. Reiter, S. Wegner, A. Purea, M. R. Wasielewski, F. De Biasi, O. Ouari, L. Emsley, **2026**, *In review*.

Flash Talk

Efficient Electron Transfer Employs High-Performance in photo-CIDNP

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[3]PRESTO, JST, Honcho 4-1-8, Kawaguchi, Saitama 332-0012, Japan
[4]CREST, JST, Honcho 4-1-8, Kawaguchi, Saitama 332-0012, Japan

Although NMR is a powerful analytical tool, its inherently low sensitivity at room temperature remains a fundamental limitation. Photo-chemically induced dynamic nuclear polarization (photo-CIDNP) addresses this by generating hyperpolarization through a cyclic reaction: photo-induced electron transfer yields a radical pair, which then undergoes nuclear-spin-selective intersystem crossing. While photo-CIDNP is highly practical, operating at room temperature under light irradiation, the achievable polarization level has typically been orders of magnitude lower than that of other hyperpolarization techniques. Continuous-wave irradiation offers a promising approach to accumulate high polarization in the steady state of this photochemical cycle. Molecular design for photo-CIDNP has predominantly focused on maximizing nuclear spin selection efficiency [1]. However, the initial electron transfer (ET) step is equally vital, as it governs the overall turnover rate of the reaction cycle.

Here, we demonstrate a novel molecular design strategy that pairs efficient ET with optimal nuclear spin selection to achieve substantial hyperpolarization. We employed a porphyrin-based cation as a strong electron-accepting dye and systematically evaluated fluorophenol derivatives as quenchers. The ^{19}F nucleus in fluorophenols provides large hyperfine coupling, ensuring highly efficient nuclear spin selection. Our transient absorption and NMR studies revealed a clear positive correlation: higher ET quantum yields from the triplet dye directly translate to higher photo-CIDNP efficiencies. By comprehensively optimizing excitation light power, external magnetic field, and sample concentrations, we recorded a 22,000-fold ^{19}F NMR signal enhancement (exceeding 10% polarization).

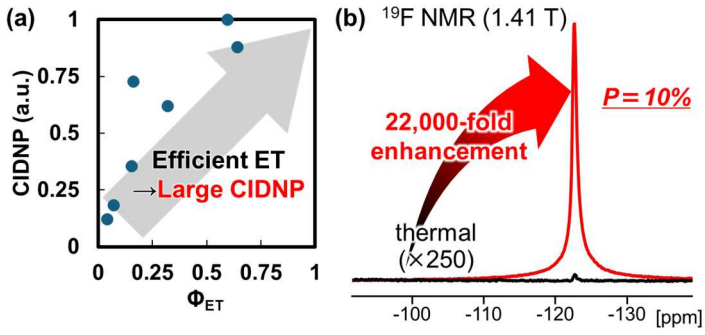


Figure 1. (a) Correlation between ET efficiency and CIDNP intensity; (b) 22,000-fold ^{19}F NMR enhancement via photo-CIDNP.

[1] F. Torres et al., *Phys. Chem. Chem. Phys*. **2021**, *23*, 6641.

Flash Talk

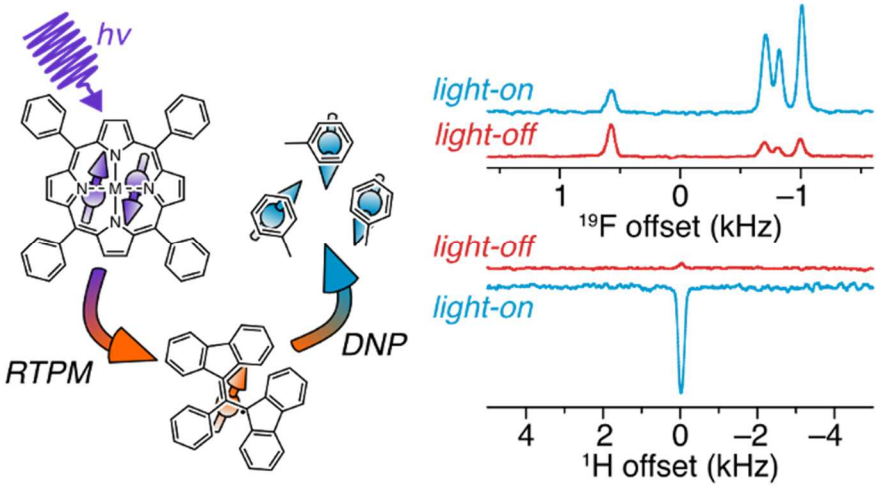
Optical hyperpolarization of ^{1}H and ^{19}F spins in organic liquids

Federico De Biasi[1], Lorenzo Franco[1], Marco Ruzzi[1], Gabriele Stevanato*[1]

[1]*Department of Chemical Sciences, University of Padova, Via Marzolo 1 35131 Padova, Italy*

Hyperpolarization methods boost nuclear spin polarization well beyond the Boltzmann limit, overcoming the intrinsic low sensitivity of NMR spectroscopy. They also accelerate multidimensional experiments and enable the observation of heteronuclei with high analytical value. Among these, ^{19}F NMR is of particular interest because of the absence of background interference and large chemical shift dispersion of ^{19}F. Dynamic nuclear polarization (DNP) remains the most widely used hyperpolarization approach for sensitivity boost in solids and liquids, where microwave radiation mediates the polarization transfer from an electron spin source to target nuclear spins.

Optical DNP (oDNP) generates non-equilibrium electron spin polarization using light rather than microwaves. In solution, this can occur through the radical–triplet pair mechanism when a photoexcited triplet chromophore interacts with a stable radical. The photoinduced electron spin polarization can then be spontaneously transferred via cross-relaxation to target nuclei, *i.e.*, via the Overhauser effect.[1] Here, we investigate porphyrin–BDPA pairs for oDNP in organic solvents using illumination from an incoherent light-emitting diode, providing ^{1}H enhancement factors in bulk solutions up to −7.5 at 0.35 T and −25 at 0.16 T.[2] Beyond ^{1}H hyperpolarization, we show optical enhancement of ^{19}F in bulk perfluorotoluene (+5 at 0.37 T), with the positive enhancement factor indicating a significant scalar contribution to the electron–nuclear interaction. The improved photostability of porphyrins enables one- and two-dimensional oDNP experiments without sample flow, and their versatile chemical tunability opens up new perspectives for future development of oDNP methodologies in liquids.



[1] M. W. Dale, and C. J. Wedge, *Chem. Commun.* **2016**, *52* (90), 13221–13224.
[2] F. De Biasi, L. Franco, M. Ruzzi, and G. Stevanato, *submitted*.

Flash Talk

Organic Diradicals Bridged by Inverted Singlet – Triplet Units for Optical – Spin Interfaces

Marco Tommaso Barreca[1], Lorenzo Savi[1], Matteo Bedogni[1], Francesco Di Maiolo[1]

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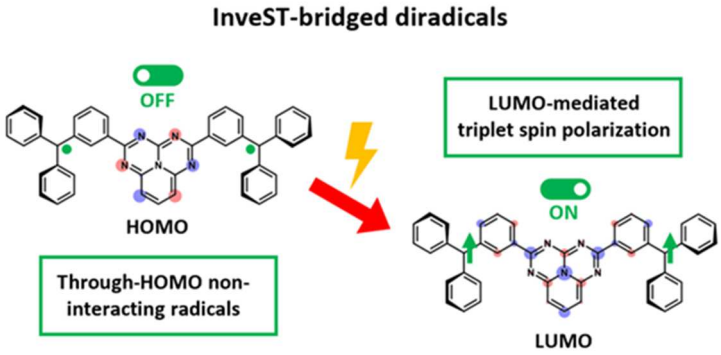
Optically addressable molecular spins are promising candidates for quantum sensing and information processing [1]. While metal-free organic diradicals offer high chemical tunability, realizing robust optically detected magnetic resonance (ODMR) functionality requires precise, light-driven control over spin-spin interactions [1].

In this talk, we present a comprehensive theoretical investigation of disjoint diradicals bridged by an inverted singlet-triplet (InveST) core. Employing the Pariser-Parr-Pople (PPP) Hamiltonian within a Restricted Active Space (RASCI) scheme, validated by multireference ab initio CASSCF/QD-NEVPT2 calculations, we demonstrate that these systems possess disjoint ground states with effectively degenerate singlet and triplet levels, indicating fully decoupled spins [2,3]. However, the population of the bridge LUMO trough optical excitation triggers a finite exchange interaction that stabilizes the triplet excited state below the corresponding singlet.

Importantly, we demonstrate that thermally accessible torsional fluctuations at the bridge-radical junctions break molecular planarity, activating spin-orbit coupling (SOC) that mediates intersystem crossing (ISC), thereby driving the robust population of the T_1 state from the excited singlet manifold and validating the proposed ODMR mechanism [2,3].

These findings highlight InveST-bridged diradicals as a robust, metal-free paradigm for room-temperature molecular qubits and spin-optical interfaces [2,3].



[1] S. M. Kopp et al. JACS 146 (2024) 27935–27945
[2] L. Savi et al. JCTC 22 (2026) 1465–1475
[3] M. T. Barreca et al. JPCA 130 (2026) 2399–2410

Flash Talk

Is there direct electron transfer from A_0 to F_X in the reaction center from *Heliobacterium modesticaldum*?

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The structures of Type I RCs found in anoxygenic bacteria show that the distance between A_0 and F_X (~18 Å) is unusually long for electron-transfer (ET) between them. The ET lifetime from A_0 to F_X in the HbRC (600-700 ps) has primarily been measured using transient-absorption (TA) spectroscopy by monitoring the A_0 signal (Chl *a*, 670 nm). However, the signal associated with F_X reduction has never been simultaneously observed at that rate, raising the hypothesis whether there is an intermediate-acceptor between A_0 and F_X. Two possibilities were considered: (1) menaquinone, playing a role analogous to that of phylloquinone in Photosystem I and (2) Y_{550}, an aromatic amino-acid with the right orientation to potentially participate in ET between A_0 and F_X. To probe the role of menaquinone, we washed the HbRC, removing 95% of quinones and observed no change in the ET lifetime. To investigate the role of Y_{550}, we used site-directed mutagenesis. HbRC-Y550M displayed minor changes in ET indicating that Y_{550} is not the secondary-acceptor. To test whether ET from A_0 to F_X is direct, mutations of residues near F_X were made. HbRC-T440V showed a longer ET lifetime and a shift in the midpoint potential of F_X (1.2 ns and -569 mV). Additionally, EPR spectroscopy revealed a S = ½ spin-state for F_X^- in HbRC-T440V. Moreover, a signal consistent with F_X^--F_X that is fully produced in 1 ns was observed by extending the detection of TA experiments into UV. Our findings prove direct ET from A_0 to F_X, i.e. F_X is the secondary-acceptor.

Flash Talk

Limits on the precision of radical pair magnetoreception in the avian retina

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Experimental evidence suggests that night migratory songbirds navigate with the help of a light-dependent magnetic compass mediated by radical pairs in cryptochrome-4a (CRY4a) proteins located in the retina [1]. We simulate two signal processing models in order to quantify the precision and accuracy with which a heading direction could be inferred from noisy flavin-tryptophan radical-pair sensors in the accessory members of double-cone photoreceptor cells. We compare a single-cell readout model (model 1) and a two-cell ratio model (model 2), designed to remove variations in light intensity and polarization. Two-cell signalling is robust under non-uniform illumination conditions that catastrophically undermine one-cell readout [2]. With an estimated magnetic anisotropy of 10^{-4}, more than 10^{10} radical pairs are required to achieve < 5° uncertainty in the inferred heading. Estimates of photon-flux for a clear moonless night suggest that at most only 10^{6} radical pairs could plausibly be created in CRY4a molecules in the retina. These results indicate that either the magnetic sensitivity of CRY4a is far larger than current theory predicts, or that compass magnetoreception in night-migratory songbirds operates by a different mechanism, not involving radical pair chemistry.

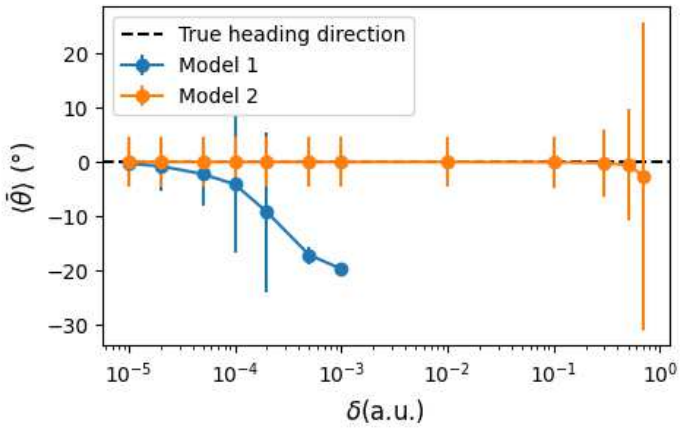

Fig. 1 Mean heading direction $\langle\underline{\theta}\rangle$ and associated uncertainty for models 1 and 2 under non-uniform illumination. The cells in the left or the right of the retina each contain 2δ times more radical pairs than the other half.

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Flash Talk

Ultrafast vibrational spectroscopy of migratory songbird cryptochrome

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The blue-light-sensitive cryptochrome proteins are the leading magnetoreceptor candidates in night-migratory songbirds. Photoexcitation of the chromophore, flavin adenine dinucleotide (FAD), followed by electron transfer (ET) along a tetrad of tryptophan residues generates a spin-correlated radical pair [1]. In FAD, nonadiabatic vibronic couplings play a key role in the initial 50-fs dynamics following photoexcitation, with theory also supporting their importance in protein [2,3], calling the applicability of Marcus theory to describe the ET into question.

Here, we perform 10-fs ultafast vibrational spectroscopy of European robin *Er*Cry4a protein and uncover pronounced evidence of nonadiabatic couplings, notably a sub-50 fs redshift in stimulated emission (quenched by ET within 0.5 ps) and a similarly rapid damping of high-frequency (> 600 cm^{-1}) vibrational modes. In contrast, low-frequency vibrations persist through both initial energy relaxation and subsequent ET with a lifetime of ~1 ps, i.e. low-frequency wavepacket motion on the excited FAD* surface is coherently transferred to the $FAD^{\bullet -}$ radical. Therefore, vibrational excitations cannot be treated as a thermal bath, as in conventional Marcus theory. Instead, both vibrational coherence during the first ET step and non-equilibrium vibrational motions of the protein backbone need to be considered to understand the structure of the radical pair, its formation, and intersystem crossing dynamics, the latter being highly relevant for understanding the spin properties of cryptochromes.

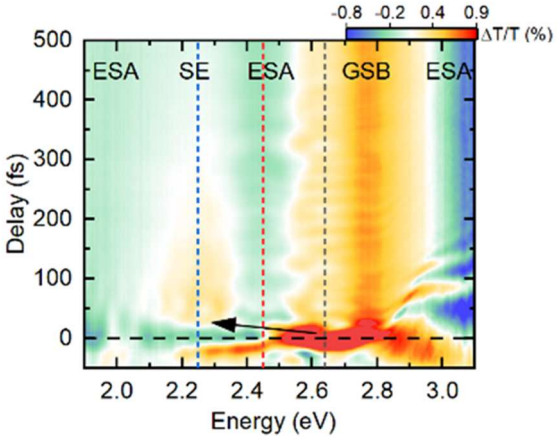

Figure 1. $\Delta T/T$ map of ErCry4a as a function of probe energy and pulse delay. Relevant ground-state bleaching (GSB), stimulated emission (SE), and excited-state absorption (ESA) transitions are marked. The black arrow indicates the rapid red-shift of the $\Delta T/T$ signal (~400 meV) during the first 50 fs.

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[3] Costa, G. J. and Liang, R. *ACS Central Science* ***11*** (**7**), 1071-1082 (2025)

Flash Talk

Separation of spin species based on echo shape for pulsed EPR

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Separation of spectrally overlapping paramagnetic species simultaneously present in a sample is often necessary in EPR in order to be able to obtain specific information on the different species. When the species differ in their total spin S, methods making use of the S-dependent transition moments can be applied. Among them is the analysis of the echo shape after application of optimised pulse sequences.

Microwave pulses in EPR are not infinitesimally short, and hence the precession around the static magnetic field $B_0$is not restricted to the time τ between the pulses. Due to the evolution of spins with $\hat{\mathcal{H}}_0 = -\gamma B_0 \hat{S}_z$ also during the applied pulses, the resulting echo shapes can deviate from the usual gaussian-like appearance and echoes can exhibit both positive as well as negative components, especially for turning angles larger than π. Upon integration over a well selected window, the obtained signal intensity can then be zero. This property can be used to spectrally separate species with different spin S, as they differ in their flip angle depending on S and m_S, and yield different echo shapes after the same pulse [1].

We were able to employ this in a project investigating gadolinium (Gd^{3+}) retention in biological samples that naturally contain a large amount of paramagnetic manganese Mn^{2+} which spectrally overlaps with Gd^{3+} even at high frequencies (W-band) [2]. We performed simulations to develop generalised pulse sequences to differentiate between the $S = 5/2$ (Mn^{2+}) and $S = 7/2$ species (Gd^3). Inhomogeneity of the microwave pulse intensity B_1 was also considered. The successful separation was shown experimentally at 94 GHz (W-band) for 2-pulse field sweep echoes (FSE) as well as 3-pulse sequences like Mims and Davies ENDOR on reference and real biological samples.

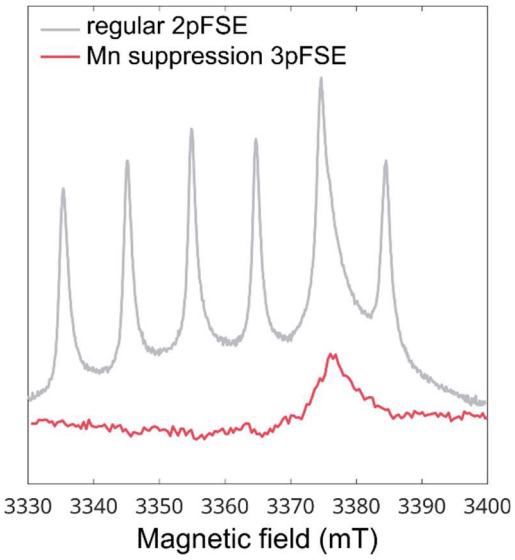

Figure 1: FSE measured on a biological sample containing Mn^{2+} and Gd^{3+}. The Gd signal is clearly visible when applying a Mn suppressing pulse sequence (red).

Support by Deutsche Forschungsgemeinschaft, CRC 1340 Matrix in Vision is gratefully acknowledged.

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Flash Talk

Laser-induced dipolar EPR combined with molecular modeling for structural studies of protein-ligand complexes

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Knowledge of binding sites in protein-ligand complexes is essential for understanding drug action and predicting off-target effects. When ligands bind transiently to the protein surface or occupy several sites simultaneously, traditional structural biology methods often fail, and computational modeling becomes necessary. Blind docking is widely used, yet incomplete conformational sampling and simplified scoring lead to substantial ambiguity, particularly when multiple sites coexist. At the same time, dipolar EPR spectroscopy provides unique access to conformational ensembles, yielding not only mean distances but also their full distributions; on its own, however, it cannot resolve the relative geometry of complex components.

We present an integrative approach combining molecular modeling with experimental EPR distance distributions to construct experimentally validated models of biomolecular complexes [1]. A single distance distribution from laser-induced magnetic dipole spectroscopy (LaserIMD) is used to filter and validate blind docking results: predicted ligand positions are clustered, filtered against the EPR data, and refined by focused docking and molecular dynamics.

The approach was applied to human serum albumin (HSA) bound to porphyrin-based photosensitizers used in photodynamic therapy. For each studied complex binding sites were obtained with great correlation with experiment. Binding-site occupancy is strongly modulated by ligand charge, size, and hydrophobicity, with photosensitizers frequently populating multiple non-canonical surface sites. Extending the scheme to multi-center EPR, combining LaserIMD, RIDME, and LITTER, we built the first all-atom experimentally derived model of the labile HSA–Chlorin e6–Cu^{2+} complex. The approach is applicable to any EPR-active ligand, including other photoactive and metal-bearing molecules.

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Flash Talk

Optimization of Magnetic Field Effects – from Magnetoreception to Biological Spin Qubits

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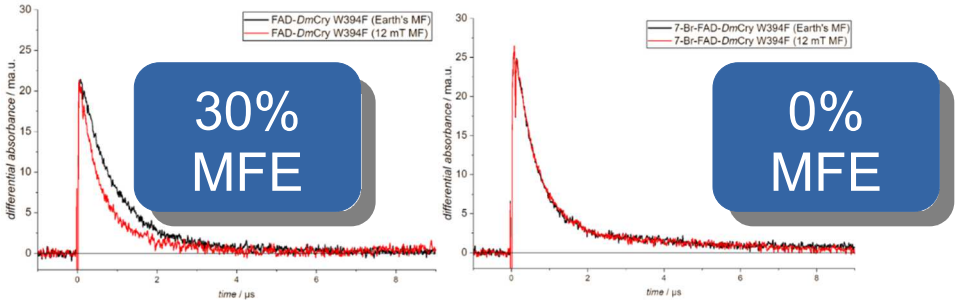
[2]*University of Freiburg, Institute of Physical Chemistry, Freiburg, Germany*

Magnetic field effects (MFEs) in spin-correlated radical pairs (SCRPs) have been studied for decades, both in solution and in more defined systems like micelles or proteins [1,2].
Recently, SCRPs in various flavoproteins – including cryptochromes – have been investigated regarding the magnetic sensitivity of their flavin emission [3,4]. A significant magnetic sensitivity was unveiled with MFEs on flavin fluorescence pushing above 30% in some variants/mutants. Such an intense modulation of emission opens the door to applications like magnetic tuning of fluorescence response *in vivo*, lock-in fluorescence detection and spin state readout via radio wave frequencies.
In my talk I will briefly outline the principles of magnetoreception via SCRPs, connect MFEs mechanistically with altered flavin fluorescence and then focus on avenues to tune the magnetic response in flavoproteins and related systems. We show that this magnetic response is governed by kinetic competition between deprotonation and direct recombination of the primary SCRP. This competition is tunable through donor identity, the protein microenvironment, and, for the first time, chemical modification of the flavin cofactor. For example, 7-fluoro modification enhances magnetic sensitivity to approx. 33% while 7-bromo derivatization leads to complete abolishment, putatively caused by a heavy atom (spin-orbit-coupling) effect [5].
Finally, time-resolved radiofrequency manipulation of a rationally designed flavin-DNA SCRP points toward coherent control and the prospect of biological spin qubits.



[1] U. E. Steiner, T. Ulrich, Chem. Rev. 1989, 89, 51–147.
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Flash Talk

Light-induced ^{1}H hyperpolarization produced by flavoprotein at 4.7 Tesla

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Photochemically induced dynamic nuclear hyperpolarization (photo-CIDNP) is a method to enhance signal intensity in NMR upon light-induced formation of spin-correlated radical pairs (SCRPs)[1]. Under solid-state conditions, using magic-angle spinning (MAS) NMR, photo-CIDNP occurring in proteins, has been limited to ^{13}C and 15N [2][3][4][5].

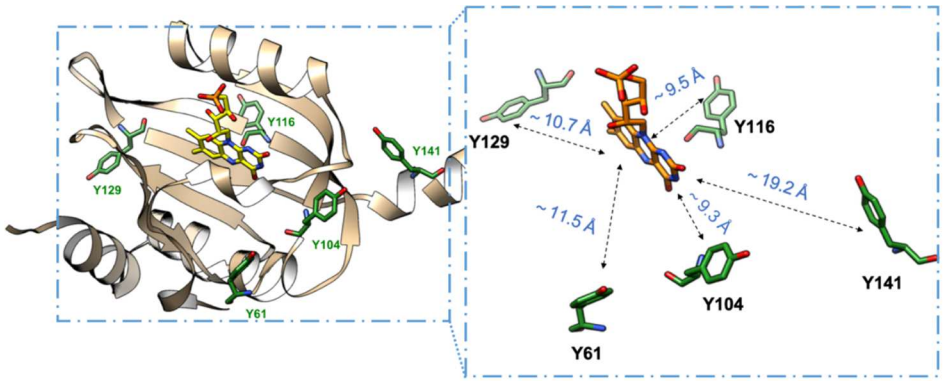

Figure 1. Structural model of the LOV domain Mr4511 with highlighting the position of tyrosine.

The light-oxygen-voltage (LOV) domain named 4511 from *Methylobacterium radiotolerans* (*Mr*4511-C71S), lacking a tryptophan, shows in a 1H MAS NMR experiment under illumination a solid-state photo-CIDNP effect at 4.7 Tesla (200 MHz 1H frequency). The light-induced 1H hyperpolarization is spreading into the aqueous buffer allowing it to be used in more generally applicable hyperpolarization strategies.

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[2] Wang X. J et al., Wuli Huaxue Xuebao/ Acta Phys. - Chim. Sin. 32, 399–404 (2016).
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Flash Talk

Probing electron transfer directionality in Far-Red PSI reaction centre by EPR spectroscopy

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The application of pulse and Time Resolved (TR) EPR spectroscopy to study photoinduced spin correlated radical pairs in Photosystem I (PSI) proved to be highly informative in understanding the electron transport (ET) pathways within its reaction centre.[1] The recent discovery of modified photosystems in organisms adapted to Far-Red light exposure[2] has revived the necessity to provide further assessments on ET in PSI in order to determine new photophysical aspects of rearranged photosynthetic complexes.

The cyanobacterium *C. thermalis* PCC7203, when exposed to Far-Red light, triggers an acclimation response (called FaRLiP) that induced the synthesis of low-energy far-red absorbing pigments (chlorophylls *d* and *f*) followed by their direct inclusion inside photosystems. Regarding PSI, the latest structural model has proposed an asymmetric localisation of a single chlorophyll *f* within the reaction centre, supposedly redirecting ET exclusively along the redox active chain of cofactors in which it is coordinated.[3]

Analysis of oop-ESEEM modulation frequencies and TR-EPR polarisation patterns applied to the $[P_{700}^{+}A_1^{-}]$ spin corelated radical pair in *C. thermalis* PSI adapted to FR light demonstrated that ET is perfectly bidirectional along the two ET branches. The asymmetric coordination of a single chlorophyll *f* molecule does not perturb the intrinsic capability of PSI to perform bidirectional electron transfer. This finding provides a framework for further discussions concerning the energetics of the reaction centre cofactors in FR-PSI.

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(3) Consoli, G.; Tufail, F.; Leong, H. F.; Viola, S.; Davis, G. A.; Rew, N.; Medranda, D.; Hofer, M.; Simpson, P.; Sandrin, M.; Chachuat, B.; Nelson, J.; Renger, T.; Murray, J. W.; Fantuzzi, A.; Rutherford, A. W. *Science* **2025**, *390* (6778). https://doi.org/10.1126/science.ado6830.

Flash Talk

Genetic encoding of non-canonical amino acids in electron transport protein complexes: moving towards protein structural determination in cellular environments using EPR

Giulia Da Ros[1], Haocheng Qianzhu[2], Kevin Hamdami[1], Vishal Bayya[3], Jack Rowbotham[1], Alice Bowen[1], Thomas Huber[2], Jeffrey Harmer[3]

[1]*Photon Science Institute and Manchester Institute of Biotechnology, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom*
[2]*Reserach School of Chemistry, Australian National University, Sullivans Creek Rd, Acton ACT 2601, Australia*
[3]*Centre of Advanced Imaging, University of Queensland, University Dr, St Lucia QLD 4067, Australia*

Structural studies of cytochrome P450 (CYPs) enzymes are currently limited by the lack of site-specific labelling methods that work in near-native conditions and that are compatible with the complex chemical environments in cells.

This project addresses this gap by developing a protocol for Gd^{3+} spin-labelling via genetically encoded non-canonical amino acids (ncAAs) and subsequent label conjugation. This enables Pulse Dipolar Spectroscopy (PDS) studies of interdomain dynamics, with the aim to improve our understanding of CYP catalytic function.

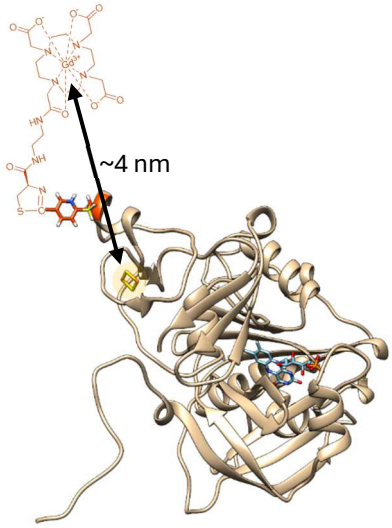

Figure 1: Cytochromes P450 CYP116B from Albidovulum Xiamenense labelled with Gd^{3+}at position A308.

Here, we apply this approach on Cytochromes P450 CYP116B from *Albidovulum Xiamenens*. Besides a heme domain, the enzymes have a reductase domain comprising ferredoxin reductase (FdR) and a single electron carrier iron-sulphur cluster ferredoxin (Fdx), exploited as a first spin centre in EPR. Efficient electron transport (ET) depends on dynamic interdomain interactions, but understanding ET regulation remains challenging because full-length structures are difficult to obtain and conventional structural methods provide only static snapshots.

To establish a cysteine-independent labelling strategy, the ncAA S-(4-cyanopyridin-2-yl)-L-cysteine (CysCNP) can be genetically incorporated and coupled to a nitrile-aminothiol (NAT) Gd^{3+} tag through bioorthogonal click chemistry, yielding a spin centre that is more resistant to reduction in cellular environments than nitroxides, previously used in CYP systems.[1,2]

PDS measurements between the Gd^{3+} tag and the native iron-sulphur cluster are used to probe distance distributions, providing specific insight into the conformational dynamics that govern ET in CYP116B.

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M. Bowen, E. O. D. Johnson, F. Mercuri, R. Qiao, J. S. O. McCullagh, J. E. Lovett, S. G. Bell, W. Zhou, C. R. Timmel, L. L. Wong and J. R. Harmer, *J. Am. Chem. Soc.*, **2018**, *140(7)*, 2514–2527#

Flash Talk

Lithium isotope effects and magnetic interactions in flavin-ascorbyl radical pairs

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For decades, lithium carbonate has been a cornerstone treatment for bipolar disorder and related conditions, yet its mechanism of action remains poorly understood.

Previous studies have suggested that the two stable isotopes, ^{6}Li and ^{7}Li, with nuclear spins of 1 and 3/2, respectively, can produce distinct biological effects. Because nuclear spin can subtly alter the course of specific chemical reactions, these studies have motivated the exploration of whether lithium's isotopes might act through a spin-dependent mechanism.

Here, we investigate the Radical Pair Mechanism in the flavin–ascorbyl system using DFT and spin-dynamics calculations. The ascorbyl radical, derived from vitamin C, is both abundant in the brain and long-lived, making it a more credible partner for flavin. We propose that lithium's nuclear spin modulates triplet yields in flavin–ascorbyl radical pairs, offering a quantum-based explanation for isotope-dependent effects. Whether these spin interactions play a clinical role remains to be determined, but the possibility is exciting and points toward a promising line of inquiry.

Flash Talk

Energy-transfer-modulated Magnetoluminescence for a five-coordinated Mn^{II} complex in organic host matrices

Takema Hikawa[1], Ryota Matsuoka[1], Asato Mizuno[1,2,3], Shojiro Kimura[4], Tetsuro Kusamoto[1,2,3,5]

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[2]*OTRI-Spin, The Univ. of Osaka, Japan*
[3]*CSRN, The Univ. of Osaka, Japan*
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Magnetic field effects on luminescence (i.e., Magnetoluminescence, MagLum) have been studied to understand correlations between spin states and luminescence in materials. Our group has reported the preparation and MagLum behaviors of a six-coordinated Mn^{II} complex doped into the solids of its Zn^{II} analogue[1]. The excited-state dynamics of the solids has been shown to involve an energy transfer (EnT) from the Zn^{II} complex to the Mn^{II} complex. The EnT process was modulated under magnetic fields to result in the MagLum at 4.2 K. Clarifying the generality of this MagLum across different molecular structures is important to expand the range of MagLum-active materials and improve the controllability for future magnetic field-sensing devices.

In this presentation, we report the preparation and photophysical properties of a five-coordinated Mn^{II} complex ($[Mn^{II}Br(SPO)_2]Br$[2], **1**) dispersed into amorphous solids of SEGPHOS oxide (**SPO**) (Figure **1a**). The photoluminescence of the **1**-dispersed solids involved an EnT process from **SPO** to **1** and was modulated under magnetic fields of up to 15 T at 4.2 K (Figure **1b**). These results were similar to those of the six-coordinated Mn^{II} complex and indicated that the EnT-modulated MagLum in Mn^{II} complexes can arise without strict limitations on molecular structures of Mn^{II} complexes or host-guest combinations. Moreover, the experimental investigations on the emission intensity and lifetime clarified that the magnetic field suppressed the efficiency of the EnT from **SPO** (host) to **1** (guest), rather than that between the adjacent **SPO** molecules.

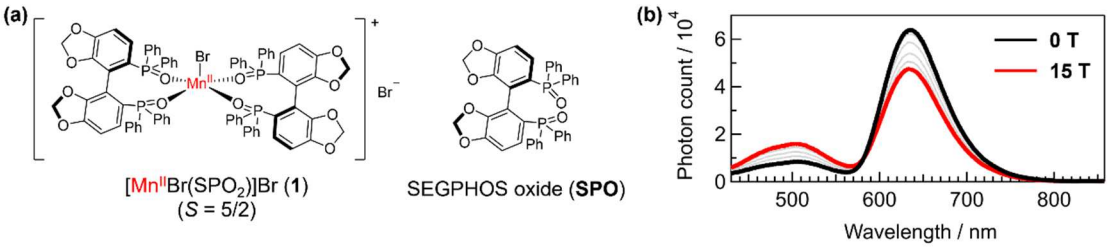

Figure 1. (a) Molecular structures of **1** and **SPO**. (b) Emission spectra of 10 mol% dispersed solid of **1** in **SPO** matrices under magnetic fileds of up to 15 T at 4.2 K (λ_{ex} = 285 nm).

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Flash Talk

Symmetry-Breaking Modulation of Platinum Sites in Multicomponent Alloy for Efficient Oxygen Reduction Reaction

Xinyi Shen[1,2], Xue Zhang[1], Wenfeng Hu[3], Xiaolin Tai[1], Wenzhi Li[1], Yuwen Chen[3], Mengzhao Zhu[1], Huijuan Zhang[1], Qinghua Zhang[4], Lin Gu[5], Yue Lin[1], Yuen Wu[1], Mei Sun*[1], Li-Ming Yang*[3], Xiaokang Liu*[1], Linlin Cao*[1], Tao Yao.*[1]

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[2]*School of Biomedical Engineering and Suzhou Institute for Advanced Research, University of Science and Technology of China, Suzhou 215123, China*
[3]*School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, Wuhan 430074, China*
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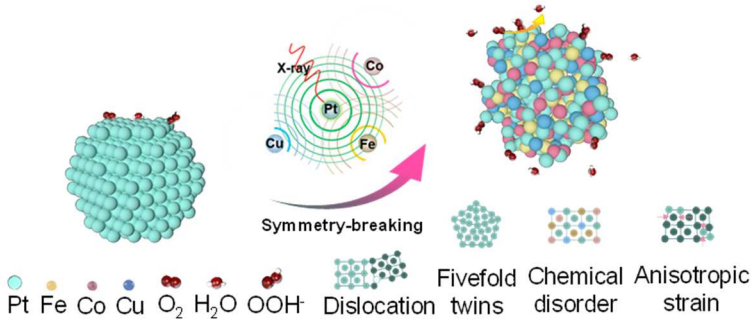
Understanding and controlling atomic-level interactions within multicomponent alloys provides a promising avenue to drive multistep tandem catalysis. Herein, we develop an atomic symmetry-breaking PtFeCoCu multicomponent alloy that disrupts long-range order and local coordination homogeneity, and identify the nature of its enhanced performance for oxygen reduction reaction (ORR). The deliberate symmetry breaking, featured by heterogeneous local coordination and anisotropic strain, enriches the Pt environment with additional transition-metal neighbors. These distortions activate multicomponent interactions and tune the Pt electronic structure, promoting ORR intermediate conversion while suppressing component dissolution. Consequently, PtFeCoCu reaches a half-wave potential of 0.95 VRHE and a mass activity of 3.53 A mg_{Pt}^{-1} at 0.9 VRHE in ORR. In an H_2-O_2 fuel cell, it delivers a high mass activity of 1.63 A mgPt-1 at 0.9 ViR-free, retaining 87.7% of its initial mass activity after 30,000 cycles. Our findings highlight symmetry breaking as a key driver with broad implications across multicomponent alloys.



[1] Reference: Angewandte Chemie International Edition, 2026.
DOI: 10.1002/anie.5938299.

Poster Abstracts

Poster Abstract

Toward Enhanced Photoluminescence in Luminescent Organic Diradicals

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Optically addressable molecular spin systems are promising alternatives to solid-state color centers, such as nitrogen-vacancy centers in diamond, for applications in quantum information science and quantum sensing. Theoretical studies by Yuen-Zhou and co-workers,[1] together with experimental studies by the groups of Wasielewski and Friend,[2–4] have demonstrated the considerable potential of luminescent diradicals consisting of two tris(2,4,6-trichlorophenyl)methyl (TTM) radicals linked through a meta-connected bridge. These diradicals exhibit spin-selective intersystem crossing between the excited triplet and singlet states, resulting in spin polarization of the ground state. As a result, such systems enable optical spin initialization and readout, as well as coherent microwave manipulation within the excited triplet levels. Further advances are expected through the incorporation of these diradicals into ordered matrices and through improvements in both phase memory time and photoluminescence quantum efficiency (PLQE). To date, achieving high PLQE in TTM diradicals remains challenging, and substantial efforts are therefore focused on the development of new TTM diradicals with enhanced luminescence efficiency.[5]

Here, we present a new modification of the TTM diradical framework, TMB-m-TTM$_2$ (Figure 1). In this diradical, both TTM units and the meta-connected bridge are functionalized with 1,3,5-trimethoxybenzene (TMB) substituents to tune the donor–acceptor properties of the TTM moieties and thereby enhance the PLQE. Indeed, TMB-m-TTM$_2$ exhibits an improved PLQE of 6.3 % (toluene, 293 K), compared with the m-TTM$_2$ and CH$_3$-m-TTM systems (0.6 % and 1.9 %, respectively, in toluene at 293 K). The optical properties of TMB-m-TTM$_2$ are investigated using UV-vis, fluorescence, and time-correlated single-photon counting spectroscopies. The EPR properties of the ground and excited states are studied by variable-temperature continuous-wave, pulsed, and time-resolved EPR spectroscopy, both in solution and in a polymethyl methacrylate (PMMA) film. The potential of TMB-m-TTM$_2$ for optical spin readout via optically detected magnetic resonance (ODMR) is currently under investigation.

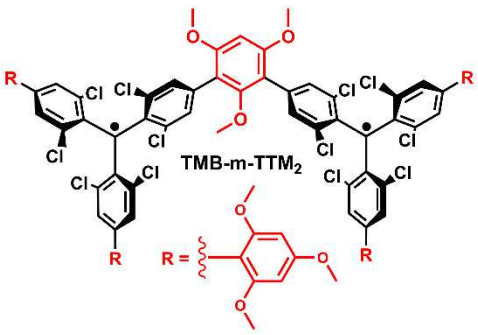

Figure 1: Structure of TMB-m-TTM$_2$.

[1] Y. R. Poh *et al.*, *J. Am. Chem. Soc.* **2024**, *146*, 15549–15561
[2] S. M. Kopp *et al.*, *J. Am. Chem. Soc.* **2024**, *146*, 27935–27945
[3] S. M. Kopp *et al.*, *J. Am. Chem. Soc.* **2025**, *147*, 22951–22960
[4] R. Chowdhury *et al.*, *Nat. Chem.* **2025**, *17*, 1410–1417
[5] M. E. Arnold *et al.*, *Chem. Sci.* **2025**, *16*, 14616–14624

Poster Abstract

ODMR reveals enhanced Carotenoid–Chlorophyll coupling and triplet quenching in Siphonous green algal Light-Harvesting Complexes

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Photostability is a fundamental requirement for photosynthetic organisms operating under variable light conditions. In light-harvesting complexes (LHCs), chlorophyll triplet states (^{3}Chl) are quenched by carotenoids through triplet-triplet energy transfer (TTET), preventing photo-oxidative damage. Although this protective mechanism has been established, the electronic principles that govern its efficiency are not fully understood. The influence of carotenoid triplet states on the chlorophyll Q_y transitions has been observed for decades in triplet-minus-singlet (T–S) absorption spectra, but the physical origin of the characteristic spectral feature in the Q_y region has remained debated. Recent combined experimental–theoretical work has clarified that this signature arises from singlet-like triplet excitations on chlorophylls perturbed by a stable carotenoid triplet [1,2], highlighting the central role of chlorophyll–carotenoid electronic coupling in both spectral modulation and fast TTET.

Here we investigate LHCs from siphonous green algae, focussing on *Codium fragile* and *Dichotomosiphon tuberosus*, which contain noncanonical carotenoids such as siphonein, siphonaxanthin, and loroxanthin. Using optically detected magnetic resonance (ODMR) alongside time-resolved EPR, we selectively probe carotenoid triplet states and their interaction with neighbouring chlorophylls. ODMR provides magnetically selective detection of ^{3}Car states, enabling unambiguous characterisation of carotenoid triplet spectra without contamination from residual unquenched ^{3}Chls. Our results reveal enhanced carotenoid–chlorophyll electronic coupling in siphonous algal LHCs, reflected in a remarkably intense Chl-Car interaction feature in the ^{3}Car T–S spectra. The strength of this feature correlates with highly efficient TTET and near-complete quenching of ^{3}Chl states. These findings show that siphonous algae implement an optimised photoprotective architecture at the molecular level, where the electronic structure of siphonaxanthin in its triplet state is shown to be at the origin of the increased coupling with nearby Chls, granting enhanced triplet quenching in these LHCs.

[1] Migliore A., Corni S., Agostini A, Carbonera D. (2023) Unravelling the electronic origin of a special feature in the triplet-minus-singlet spectra of carotenoids in natural photosystems. PCCP 25:28998-29016.
[2] Agostini A., Seki S., Calcinoni A., Paul L., Migliore A., Fujii R., Carbonera D. (2025) Siphonein enables an effective photoprotective triplet-quenching mechanism in green algal light-harvesting complexes. Cell Reports Physical Science 6(10): 102873.

Poster Abstract

Investigating the Effects of Deuteration and Host Matrix on the Spin Dynamics of Photogenerated PDI-BDPA

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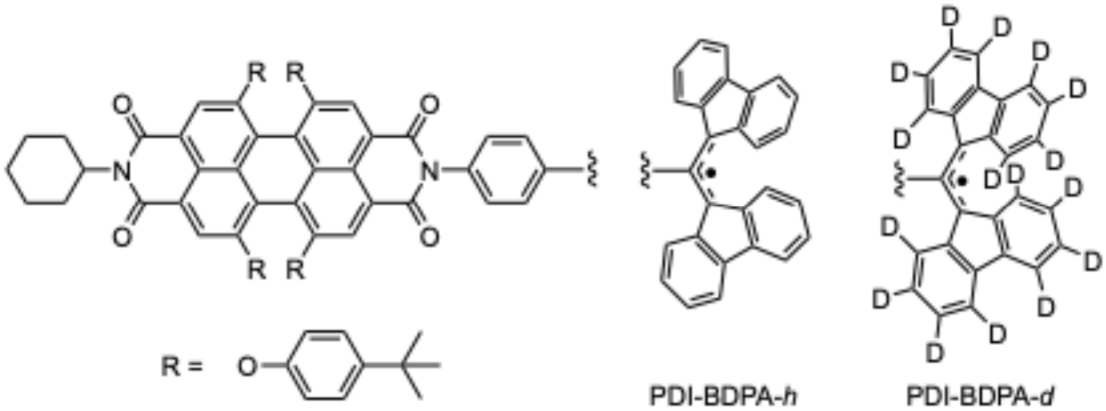
Photogenerated molecular high-spin systems, including triplet, quartet, and quintet states, have recently been proposed as a novel platform for quantum information science (QIS) [1]. These systems allow for the optical initialization and readout of quantum states, offering a distinct advantage in terms of spatial resolution and initialization fidelity. Within this context, the chromophore-radical hybrid system composed of perylenediimide and α,γ-bisdiphenylene-β-phenylallyl radical (**PDI-BDPA**) stands out as a highly viable candidate. This system is particularly renowned for its efficient spin polarization via radical-enhanced intersystem crossing and its remarkably narrow linewidth [2], which is a critical prerequisite for high-fidelity quantum operations. However, to fully realize its potential in quantum computing or sensing, a deeper understanding of its spin dynamics and decoherence pathways is essential.

In this work, we systematically investigate the impacts of chemical modification and environmental factors on the physical properties of PDI-BDPA. Specifically, we focus on the effects of deuteration of the BDPA radical and variations of matrix. We are currently evaluating their electron paramagnetic resonance (EPR) line shapes, spin-lattice relaxation lifetimes (T_1), and phase coherence times (T_2). In this presentation, we will report our ongoing experimental findings and discuss how isotopic substitution and matrix condition can be utilized to control the spin dynamics of molecular high-spin qubits.



[1] Quintes, T.; Mayländer, M.; Richert, S. *Nat. Rev. Chem.* **2023**, *7*, 75–90.
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Poster Abstract

Unifying Spin Dynamics for Magnetic Resonance: High-Performance Simulations and Analysis via Web-Based Toolkit

Irina S. Anisimova[1], Pedro H. Alvarez[1], Vladimir Bačić[1], Augusto F. Oliveira[1], Georg Langebrake[1], Luca Gerhards[1], Ilia A. Solov'yov[1]

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Spin-dependent phenomena are investigated in a wide range of magnetic resonance experiments (see e.g., EPR, photo-CIDNP, MARY, RYDMR) [1-4]. The theoretical interpretation of these experiments is becoming increasingly demanding due to the diversity of the experimental methodologies employed and the complexity of the underlying systems under study. To address these challenges, we have developed a generalized computational toolkit designed to encompass a broad spectrum of magnetic resonance techniques. Our methodology couples a quantum spin-dynamics engine, implemented in the MolSpin [5,6] program, with the web-based simulation and analysis platform VIKING [7] (www.viking-suite.com). The theoretical foundation of MolSpin is rooted in the density matrix formalism, which affords a high degree of flexibility for describing kinetic processes, relaxation phenomena, and a wide range of observables. VIKING, in turn, offers a user-friendly graphical interface, fully automated one-click submission and execution of simulations, seamless access to high-performance computing resources, and on-the-fly visualization and analysis of the resulting data.

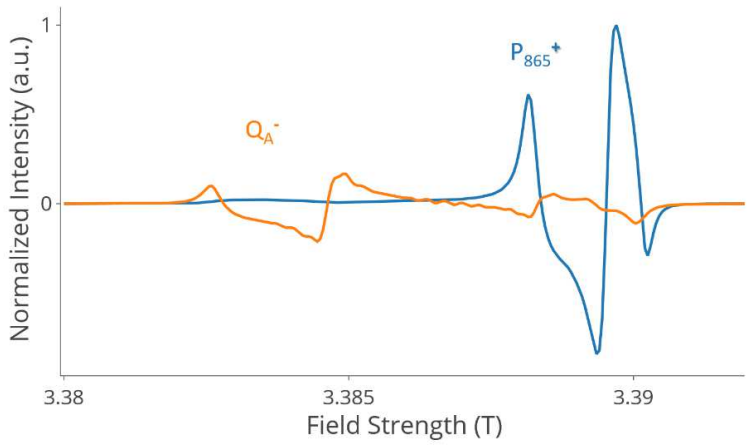

Fig.1 Simulated EPR spectra of the bacterial reaction center of *Rhodobacter sphaeroides* spin correlated radical pair $P865^{\bullet+}$–$QA^{\bullet-}$. Simulation parameters were taken from [1].

[1] C.E. Tait, *et al*., JMRO **349**, 107410 (2023).
[2] Y. Ding, A. S. Kiryutin, A. V. Yurkovskaya, *et al*., Sci. Rep., **9**, 18436 (2019).
[3] P. Mentzel, *et al*., J. Am. Chem. Soc. **147**, 26, 23068–23078 (2025).
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[7] V. Korol, P. Husen, E. Sjulstok, et al., ACS Omega, **5**, 1254–1260 (2020).

Poster Abstract

Influence of the radical properties in triplet–radical spin-polarization transfer

Dominic Bruyers[1,3], Ashley Redman[1,3], Gilles Casano[2], Soléyah Houguet[2], Sebastien Gauden[2], Olivier Ouari[2], Stefan Weber[1], Sabine Richert[3]

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[3]*University of Ulm, Institute of Physical Chemistry II, Ulm, Germany*

The generation of non-equilibrium electron spin polarization represents a key strategy for enhancing sensitivity in electron paramagnetic resonance (EPR) and nuclear magnetic resonance (NMR) spectroscopy [1]. The radical triplet pair mechanism (RTPM) enables highly efficient transfer of polarization, generated via photoexcitation of a chromophore with high triplet yield, onto stable radicals in liquid solution [1]. While the mechanism behind chemically induced dynamic electron polarization (CIDEP), and environmental influences such as temperature, viscosity, and pH are well established [1, 2], properties of the stable radicals have not yet been examined in detail.

In this study, we systematically investigate how the molecular structure and relaxation dynamics of nitroxide radicals influence the CIDEP [2,3]. A series of structurally modified nitroxide radicals, based on TEMPOL (4-Hydroxy-2,2,6,6-tetramethylpiperidinyloxyl), was examined in the presence of rose bengal as a photosensitizer, see **Figure 1**. The modification included deuteration and successive increase in the steric demand of substituents close to the nitroxide moiety. Spin polarization was characterized using transient EPR (trEPR) and pulse EPR methods at X- and Q-band frequencies under air-saturated conditions.

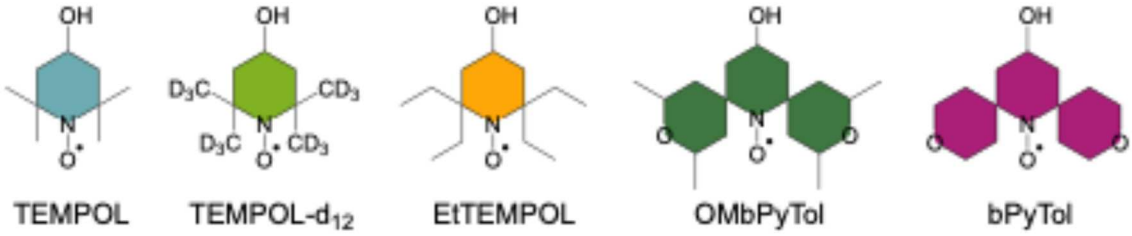

Figure 1: Structures and trivial names of the investigated nitroxide stable radicals.

The results suggest that polarization efficiency is primarily governed by the interplay between spin–lattice relaxation time (T_1) and steric accessibility of the nitroxide moiety. While longer T_1 times were generally correlated with higher polarization, steric shielding seems to significantly reduce the observed polarizations. These findings provide important design guidelines for the development of optimized polarization agents for future hyperpolarization applications under ambient conditions in liquid solution.

[1] Kawai, A. *Appl. Magn. Reson.* **2003**, *23*, 349–367.
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Poster Abstract

Singlet Fission in H/J Diketopyrrolopyrrole Aggregates under the Gaze of Time Resolved Optical and Magnetic Spectroscopy

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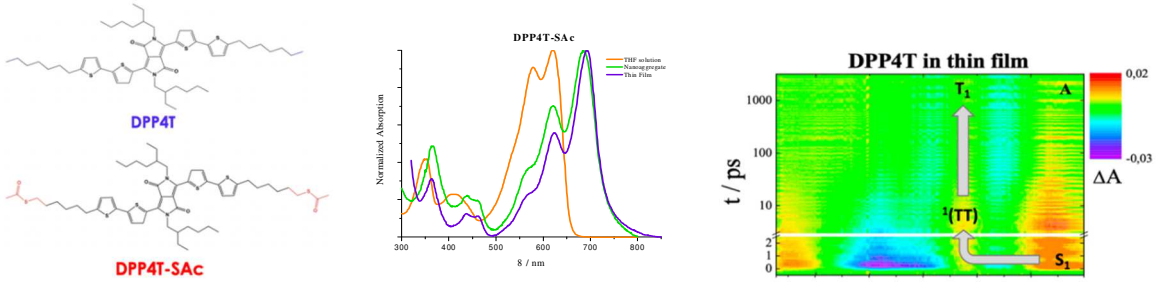
In this work, the phenomenon of singlet fission (SF), interesting for its potential applications in organic photovoltaics, photodynamic therapy and quantum information science, has been studied. We explored the aggregation effect on intermolecular Singlet Fission[1] for two diketopyrrolopyrrole derivatives differently functionalized[2], with methyl or thioacetyl groups. The different molecular structure enabled control of the supramolecular aggregation and SF activation by selecting different aggregate configurations. To this aim we prepared nanoaggregates in water dispersion, which could be interesting for photodynamic therapy applications, and solid state thin films, potentially exploitable for photovoltaics and quantum information science.

The first evidence of SF activation was the huge aggregation-induced fluorescence quenching, with a drop in the fluorescence quantum yields from solution to aggregated media, and a shortening of the fluorescence lifetimes. This raised the possibility that another deactivation pathway could be activated, possibly SF. Moreover, while in solution no triplets were produced by direct excitation, in aggregated media efficient triplet formation was observed through ns-Transient Absorption (TA). fs-TA revealed the activation of aggregation induced SF: peculiar rise-decay-rise kinetics were observed only in correspondence of the J-aggregate ground state bleaching, proving the consumption of ground state over tens to hundreds of ps, caused by the interaction between S_1 and S_0 to form the double triplet state. By tuning the excitation wavelength and the molecular structure, it was possible to evaluate the SF efficiency and rate by selectively exciting H or J aggregates. Time-resolved Electron Paramagnetic Resonance (trEPR) experiments effectively assessed the formation of triplets via SF and of the quintet multiexcitonic intermediate in thin films.



[1] R. Cantoni, M. Alebardi, E. M. D'Amato, C. Popli, Y. Patil, P. Mancini, A. Di Michele, A. Spalletti, R. Misra, T. Goodson, B. Carlotti, Adv. Funct. Materials, 2025, e17911.
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Poster Abstract

Spin Polarisation of Gadolinium Complexes by Photoexcited Rhenium Chromophores

Jonathon Clark[a,b], Hannah Eckvahl[a,b], Matthew Allen[b], Gabriel Moise[a, b], Tom Mosseri[a,b], Stephen Faulkner[b], Christiane Timmel[a,b]

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Optical initialisation remains one of the most promising avenues for the practical implementation of qubits and qudits based on molecular spin centres, allowing for generation of a (theoretically) well-defined spin state. While optical initialisation has been demonstrated in both organic and inorganic systems, its application to lanthanide-containing complexes has only recently emerged.[1] Lanthanide complexes are particularly attractive candidates for molecular spin qudits (qubits with S > 1/2), combining long coherence times with stable high-spin ground states due to the contracted nature of the 4f-electrons. Qudits have exciting potential in quantum information science, enabling more efficient quantum algorithms and providing opportunities for error-correction schemes. We recently demonstrated that photoexcitation of a neighbouring organic chromophore led to spin polarisation of the ground state of a Gd^{3+} ion.[1] To optimise systems for future applications, we proposed using coordination chemistry, instead of covalently attaching the chromophore to the lanthanide complex, to screen chromophores and lanthanide environments more efficiently. Initially we used a combination of optical, cw- and pulsed EPR spectroscopies to characterise the binding of a chromophore bearing a pendant carboxylate to a lanthanide complex, Figure 1. For the chromophore we decided to explore Re(I) complexes as they are known to have high molar absorption coefficients and readily form strongly emissive ^{3}MLCT states upon photoexcitation. We then employed trEPR to explore the spin-polarisation of the Re(I) triplet state, and the factors which affect the induced spin polarisation of a Gd^{3+} ground state.

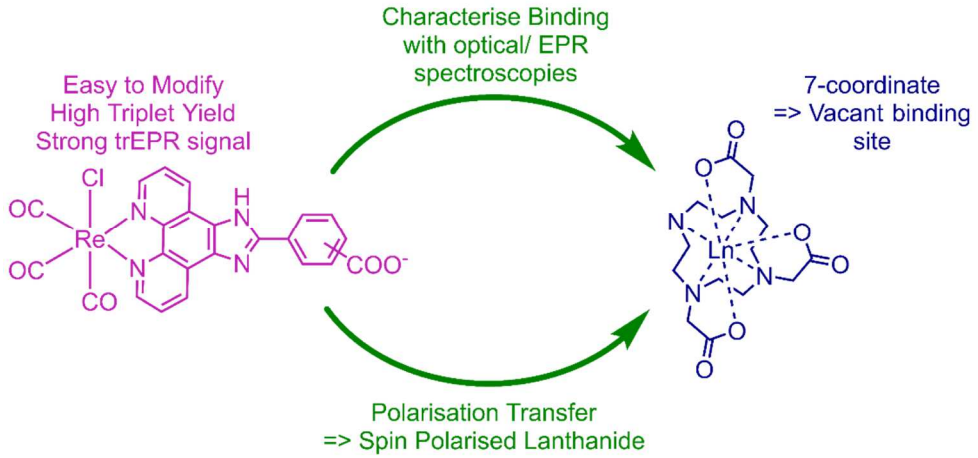

Figure 1. The Re(I) chromophore and lanthanide complex chosen for study in this project.

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Poster Abstract

Molecular Alignment in Liquid Crystals for Improving Gate Fidelity in Molecular Electron Spin Qubits

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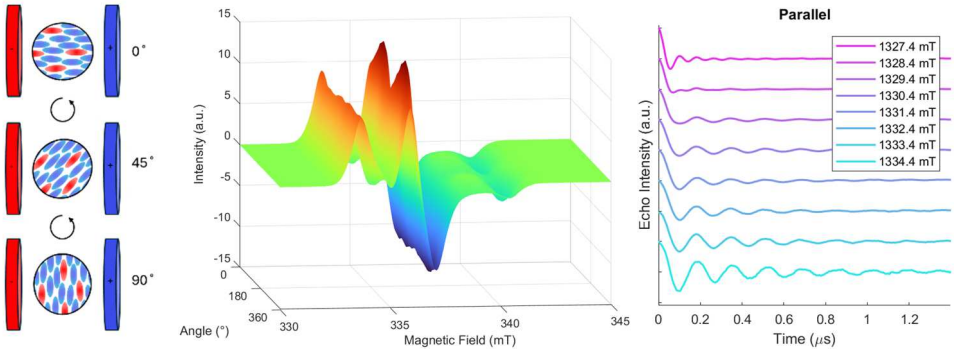
For decades, quantum technology has promised vast improvements in the amount of computational power and time required to carry out calculations for which quantum algorithms can be found.[1] These include applications such as cryptography (Shor's algorithm), database searching (Grover's algorithm) and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

MESQs employ the two spin states of an unpaired electron, which can be manipulated using microwave pulses, and measured by EPR spectroscopy apparatus. Their potential benefits over alternative implementations include tunability through molecular design, relatively high-temperature use and long phase coherence times. Previous research has suggested that molecular alignment of candidate systems should improve quantum gate fidelities.[2]

In this work we explore the use of liquid crystals to align molecules and characterize the impact of restricting molecular orientations using an alignment matrix on the distribution of dipolar coupling frequencies. Frozen solution continuous wave EPR and orientationally-selective Double Electron-Electron Resonance (DEER) measurements are used to compare ordered to disordered samples.[3]



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Poster Abstract

Avian Cryptochrome Photochemistry: Sensing vs Signalling

Daniel Cubbin[1], Tommy Pitcher[1], Chloe Archer[1], Jiahan Zhao[1], Carl Olavesen[1], Lewis Antill[1], Kevin Henbest[1], Rabea Bartölke[2], Jessica Schmidt[2], Henrik Mouritsen[2], Peter Hore[1], Christiane Timmel[1], Stuart Mackenzie[1]

[1]Department of Chemistry, Chemistry Research Laboratory, University of Oxford, OX1 2TA
[2]AG Neurosensory Sciences/Animal Navigation, Institut für Biologie und Umweltwissenschaften, Carl-von-Ossietzky Universität Oldenburg, Oldenburg

Certain bird species are known to use the Earth's magnetic field for long-range migration, a phenomenon known as magnetoreception. While the underlying biophysical mechanism remains contested, one leading hypothesis is the radical pair mechanism (RPM). Originally proposed in the context of migration by Schulten *et al*.[1], the RPM relies on the spin dynamics of spin-correlated radical pairs (SCRPs) to function as a biological compass. Cryptochrome proteins in the avian retina are currently the prime candidate for hosting such a process.

A tetrad of highly conserved tryptophan residues, and possibly a terminal tyrosine residue, are crucial for SCRP formation within avian cryptochromes. Upon photoexcitation of the FAD chromophore, these amino acids facilitate an electron transfer cascade, spatially separating the radicals involved. Here we investigate how mutating these residues affects the cascade and hence the magnetic field effect (MFE) in the protein. Measurements on these mutant proteins demonstrate that, for the mutations investigated, the greater the deviation from the wildtype (WT) sequence, the more sensitive it is to magnetic fields on the microsecond timescale.

To act as a biological compass, a cryptochrome protein must not only sense the magnetic field but also signal that information to the bird's brain. To rationalise the counterintuitive MFE results, irradiation experiments spanning from minutes to hours were conducted to quantify the rates of production of the long-lived $FADH^{\bullet/-}$ photoproducts, believed to be the signalling state within avian cryptochromes. Our results suggest a trade-off between magnetic sensitivity and the efficient generation of the signalling state.

[1] K. Schulten, et al. "A biomagnetic sensory mechanism based on magnetic field modulated coherent electron spin motion," Z. Phys. Chem. (N F), vol. 111, pp. 1–5, Jan. 1978.
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Poster Abstract

Investigating Secondary Polarization Transfer in Flv-Pro$_n$-Trp Diads by Liquid-State ^{1}H Photo-CIDNP NMR

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[2] *Universität Leipzig, Institut für Organische Chemie*
[3]*Carl von Ossietzky Universität Oldenburg, Institut für Physik*

Photochemically induced dynamic nuclear polarization (photo-CIDNP) is a hyperpolarization technique for investigation of radical-pair processes in photoactive molecular systems. Flavin-tryptophan donor-acceptor systems are widely used as model systems for studying the influence of molecular structure on photo-CIDNP signal generation [1]. Our group previously developed a series of biomimetic flavin-polyproline-tryptophan diads, Flv-(Pro)$_n$-Trp, with a donor-acceptor separation controlled by a polyproline linker [2, 3].

Previous studies on these systems revealed unexpected photo-CIDNP signals originating from proline residues, despite proline not participating directly in the formation of the primary spin-correlated radical pair [2]. This observation had suggested the presence of a secondary polarization transfer pathways.

In the present work, we investigate the origin of proline polarization using a liquid-state ^{1}H photo-CIDNP NMR spectroscopy, selective 1D ROESY experiments, concentration-dependent measurements, and after illumination delay studies. ROESY experiments revealed a spatial proximity between proline and flavin protons, while no corresponding contacts between proline and tryptophan are observed. The observed concentration and linker-length dependences further support an intramolecular origin of the effect.

The results are consistent with a model in which polarization is generated within the primary flavin-tryptophan radical pair and subsequently transferred to proline nuclei via secondary intramolecular processes, most likely mediated by cross-relaxation. These findings provide a new insight into spin-polarization transport in covalently linked photo-active donor-acceptor systems.

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Poster Abstract

Bimetallic Lanthanide Complexes as Tuneable Molecular Spin Qubit Candidates

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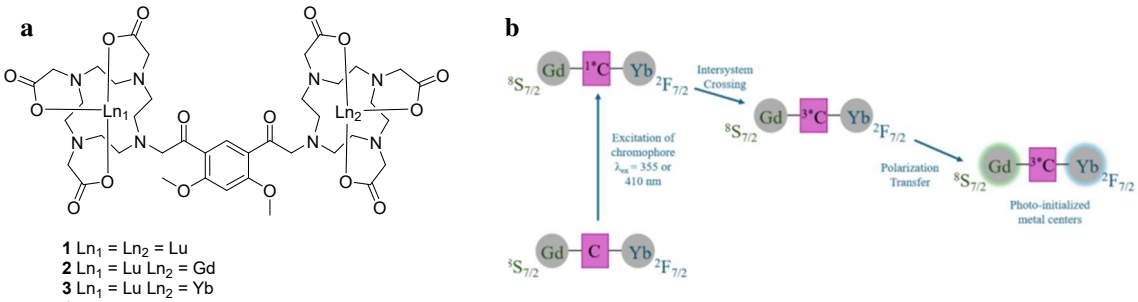
Lanthanide complexes are promising qubit candidates owing to their synthetic tunability and stable high spin states. Gadolinium, in particular, has an S = 7/2 spin state, potentially allowing for more complex computation and the quantum error correction.[1] Recently, the Timmel group demonstrated polarisation of the S = 7/2 spin state of Gadolinium by magnetically coupling it to the excited triplet state of a covalently attached organic chromophore.[2] This demonstrates the ability to initialise it into a well-defined quantum state, one of seven criteria for the physical implementation of qubits as laid out by DiVincenzo.[3] While this is a good start, to fully realise the physical implementation of qubits, a complete set gate operations will be necessary; this requires at least two coupled qubits.[3] To this end, one bimetallic complex has been synthesized and characterized and five further complexes (**1** and **2-5**, respectively, Figure 1) will be synthesized and characterised to understand their photophysical and spin properties. In complex **1**, both metal centres are lutetium, which is diamagnetic and thus provides an effective spin-free control. Preliminary experiments demonstrated that selective photoexcitation of the central chromophore generates an excited triplet state via intersystem crossing. Further work will be done to understand how this triplet state will interact with the paramagnetic metal centres in complexes **4-6**. To aid in this analysis, complexes **2** and **3** will serve as monometallic controls. Experiments to be done include CW and time resolved EPR, steady state optical absorption and emission experiments, and transient absorption and time correlated single photon counting (TCSPC).



1 $Ln_1 = Ln_2 = Lu$
2 $Ln_1 = Lu$ $Ln_2 = Gd$
3 $Ln_1 = Lu$ $Ln_2 = Yb$
4 $Ln_1 = Ln_2 = Gd$
5 $Ln_1 = Ln_2 = Yb$
6 $Ln_1 = Gd$ $Ln_2 = Yb$

***Figure 1. a**. Bimetallic complexes **4**, **5**, and **6** and control complexes **1**, **2**, and **3**. **b.** Proposed photoscheme of polarisation of the lanthanide qubits.*

[1] S. Lim, J. Liu and A. Ardavan, *Physical Review A* **2023**, *108*, 062403.
[2] J. I. Clark, K. Henbest, D. Frantzov, A. Stuhec, D. Kovacs, A. J. Redman, C. R. Timmel and S. Faulkner, *J. Am. Chem. Soc.* **2026**, *148*, 11438–11444.
[3] D. P. DiVincenzo, *Fortschritte der Physik* **2000**, *48*, 771–783.

Poster Abstract

BisNHC-Rhodium Complexes for Parahydrogen Induced Polarization

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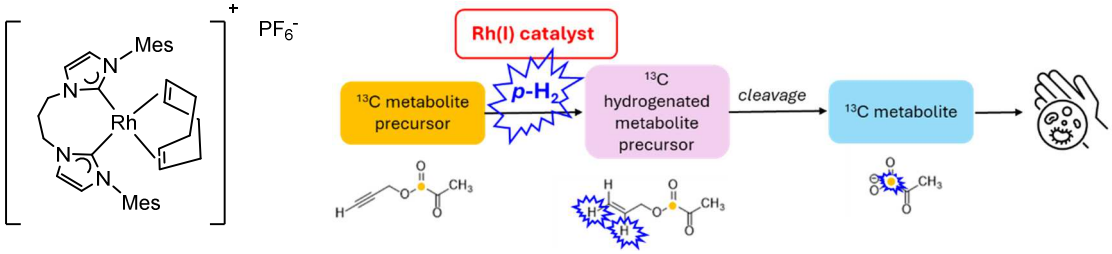
PHIP hydrogenation is traditionally dominated by rhodium catalysts bearing chelating diphosphine ligands, which efficiently promote pairwise parahydrogen addition and generate high levels of nuclear spin polarization.[1] These catalysts are also central to PHIP-SAH approaches for pyruvate [2], where polarization is introduced through hydrogenation of an unsaturated ester side arm and subsequently transferred to the ^{13}C-labelled pyruvate moiety before side-arm cleavage. BisNHC-rhodium(I) complexes represent an unexplored class of catalysts for parahydrogen-induced polarization (PHIP). Their strong σ-donating character should favour H_2 oxidative addition, although activation of the corresponding cyclooctadiene precursors is strongly limited by inefficient COD removal. Among a series of [BisNHCRh(COD)]PF_6 complexes, a mesityl-substituted derivative bearing a three-methylene linker showed the highest activity and was selected for further investigation. In the hydrogenation of our PHIP-SAH precursor, the BisNHC system generated lower initial ^{1}H hyperpolarization than the benchmark diphosphine catalyst, reaching approximately 3% polarization compared with about 10% for [Rh(dppb)COD]BF_4. Interestingly, after polarization transfer to ^{13}C by means of a field-cycling procedure, the ^{13}C hyperpolarization measured on a 60 MHz benchtop NMR spectrometer was comparable to that obtained with the diphosphine benchmark. This apparent discrepancy may arise from a longer ^{13}C T_1 in the presence of the BisNHC catalyst, which could allow more efficient preservation of the transferred polarization during the field-cycling sequence and subsequent detection. Parahydrogen enhanced NMR experiments also provided direct evidence that the BisNHC complex activates H_2 through oxidative addition, leading to the formation of Rh(III) hydride intermediates. Experimental observations were therefore combined with DFT calculations to clarify the activation pathway and provide mechanistic insight into this previously unexplored class of PHIP catalysts.



[1] J. Eills et al., Chem. Rev. 2023, 123, 1417–1551
[2] F. Reineri, T. Boi and S. Aime, Nat. Commun. 2015, 6, 5858

Poster Abstract

Unravelling the Photocatalytic Mechanism of a BODIPY–Rhenium CO_2 Reduction Photocatalyst by EPR Spectroscopy

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The increasing concentration of atmospheric CO_2 and its contribution to global warming motivate the research for efficient CO_2 conversion strategies. Photocatalytic reduction of CO_2 to value-added products such as CO has attracted considerable attention. Despite rhenium carbonyl complexes coupled to organic photosensitisers having emerged as promising molecular catalysts for CO_2 reduction [1], understanding of the photocatalytic mechanism and of the molecular properties required for increased photocatalytic activity remains limited.

In this work, we investigate the initial steps of the photocatalytic mechanism in anthracene- and phenyl-functionalized BODIPY-rhenium bipyridine photocatalysts by EPR spectroscopy. Transient electron paramagnetic resonance (trEPR) probes the triplet state formed by ISC following photoexcitation. Continuous-wave EPR (CW-EPR) under continuous illumination reveals subsequent radical formation on a much slower timescale. By comparing the behaviour of the full photocatalyst with that of its isolated molecular building blocks, this work aims to clarify the role of the different constituents in determining triplet-state formation and character as well as the electron transfer in solution, ultimately influencing the efficiency of photocatalytic CO_2 reduction.

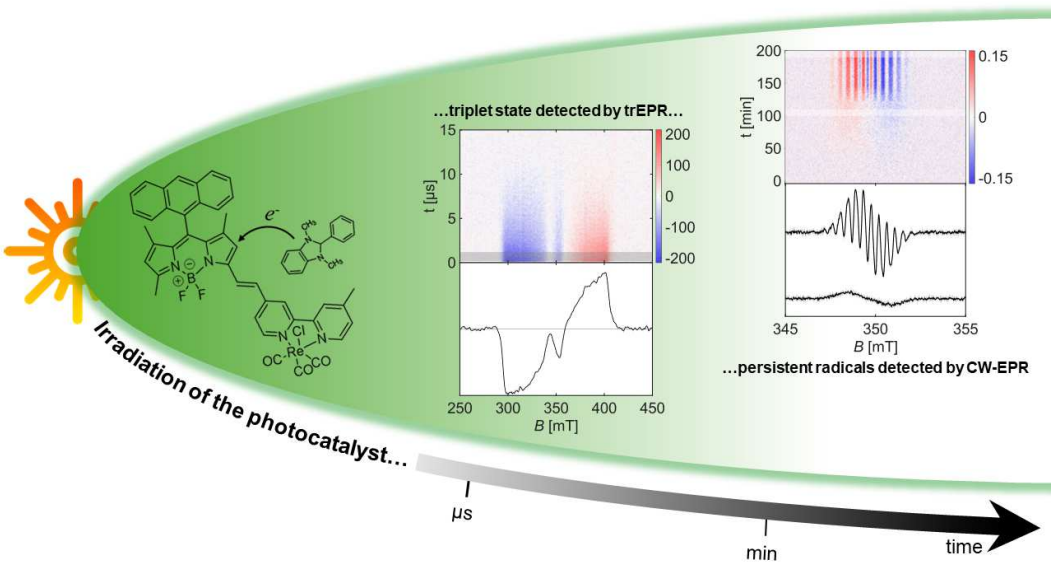

Figure 2. Overview of the photocatalytic activation of a BODIPY-based Re complex monitored by triplet trEPR measurements at 80 K and RT CW-EPR detection of persistent radical species.

[1] K. Kamogawa, Y. Kato, Y. Tamaki, T. Noguchi, K. Nozaki, T. Nakagawa, O. Ishitani, Chem. Sci., 2024, 15, 2074.

Poster Abstract

Towards Fully Automated Benchtop NMR: An Integrated System for Hyperpolarization and Optical Polarization

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Nuclear Magnetic Resonance (NMR) spectroscopy stands as a cornerstone analytical technique, yet its utility is fundamentally constrained by inherently low sensitivity, which hinders the study of fast chemical dynamics, dilute analytes, and short-lived intermediates. Hyperpolarization techniques — including optical pumping, photochemical approaches, parahydrogen-induced polarization, and dynamic nuclear polarization (DNP)—offer orders-of-magnitude signal gains, but their successful implementation demands exquisite temporal coordination among sample preparation, light delivery, and magnetic resonance detection. To address this challenge, we present a fully automated control system for a benchtop NMR spectrometer that seamlessly orchestrates hyperpolarization and optical polarization experiments. At the heart of the system lies a stepper-motor-driven sample handler, which accurately positions a sealed 5 mm NMR tube within the spectrometer bore, while a 405 nm LASER or ultraviolet source, coupled to a cylindrical lens assembly, produces a uniform vertical beam profile for homogeneous illumination across the entire 5 cm sample column. Crucially, the automated sequence—encompassing precise laser exposure, motorized sample transfer, and TTL-triggered NMR acquisition—operates with a sample transit time of approximately 0.73 s from the illuminated region to the detection zone, ensuring minimal polarization decay during transfer. The setup is fully compatible with both parahydrogen-based hyperpolarization and optical DNP experiments, as well as the automation sequence—comprising laser exposure, motor-controlled sample insertion and removal, and TTL-triggered NMR acquisition—is executed repeatedly for a user-defined number of cycles (N), enables robust signal averaging and real-time kinetic monitoring of evolving chemical systems.

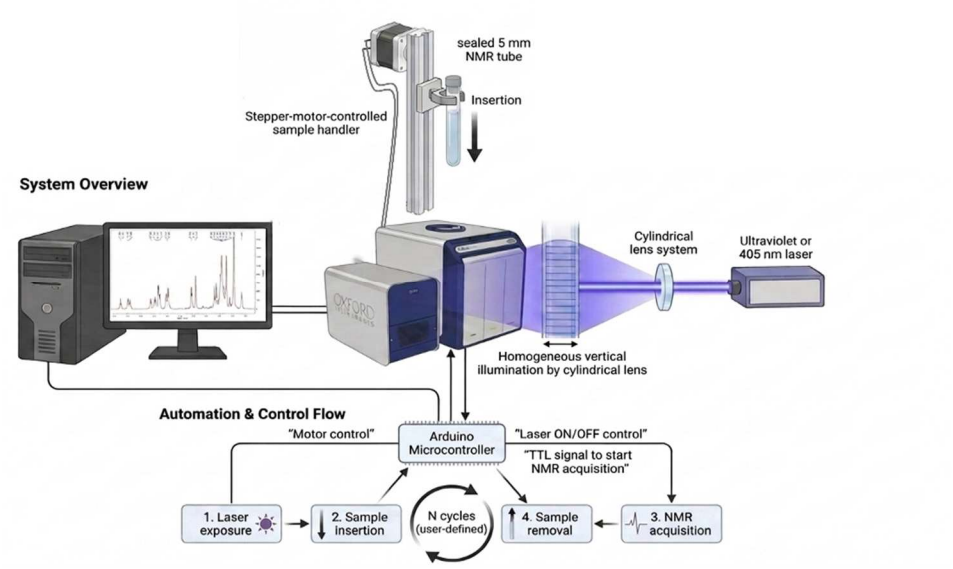

Fig 1. Schematic representation of fully automated experiment: precise synchronization of light, sample, and acquisition.

Poster Abstract

Investigation of Spin Dependent Processes in Polymer-Fullerene Organic Solar Cells by Pulsed EDMR.

Assunta S. Felice[1], Lorenzo Catini[1], Claudia Tait[1]

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Organic solar cells (OSCs) based on bulk-heterojunction donor-acceptor blends provide a versatile, low-cost photovoltaic platform with high molecular tunability. Following photoexcitation, excitons diffuse to the donor–acceptor interface, where charge separation and carrier extraction generate photocurrent. In this work, we probe spin states governing current generation in miniature polymer-fullerene solar cells via Electrically Detected Magnetic Resonance (EDMR) spectroscopy at cryogenic temperatures.

Pulsed EDMR detects spin states involved in spin-dependent processes by monitoring transient photocurrent changes following a microwave π pulse [1]. Combined with field-dependent Rabi nutation experiments, this yields information on spin states and the nature of spin-dependent processes. Variations in EDMR transient behaviour and associated spectral line shape changes across blends with different polymer donors prompted a time-resolved analysis of Rabi nutation experiments (Fig.1). Distinct spin-state contributions were identified at early and late times following the microwave pulse, reflecting differences in the underlying spin-dependent kinetics [2]. Introducing this temporal dimension to pulsed EDMR measurements, alongside spectral deconvolution, reveals kinetic behaviour beyond that expected from bipolar recombination alone.

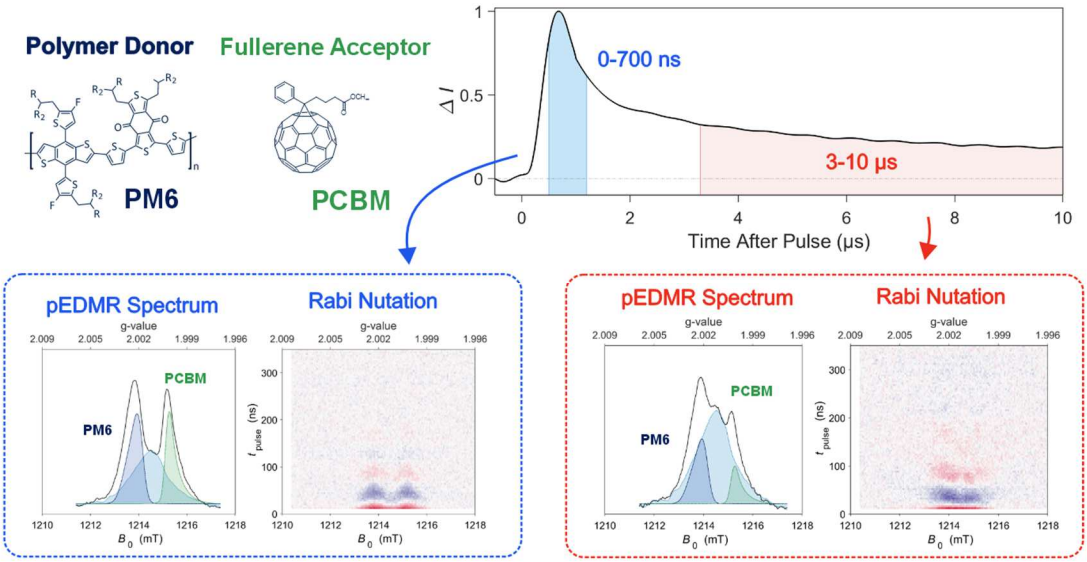

Fig 1: pEDMR spectra and corresponding Rabi nutations obtained from short- and long-time integration windows of the current transient.

[1] A. Schnegg et al., Phys. Chem. Chem. Phys., 2012, 14, 14418–14438.
[2] C. Boehme and H. Malissa, eMagRes, 6, 2017 83-100

Poster Abstract

Magnetic High Field Effects in Chalcogen Substituted NDI Donor-Acceptor Dyads

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[1]*University of Würzburg*

Following photoexcitation of rigidly linked donor-acceptor dyads, charge separation leads to the formation of spin correlated radical pairs whose lifetime can be modulated by applying an external magnetic field. Previous work has demonstrated pronounced high-field effects in dyads containing a 1,7 chalcogen substituted perylene acceptor, which was attributed to *g*-tensor anisotropy relaxation effects at high magnetic fields.[1] In this work, the perylene core of the acceptor was replaced with a naphthalene-based structure (Fig. 1).

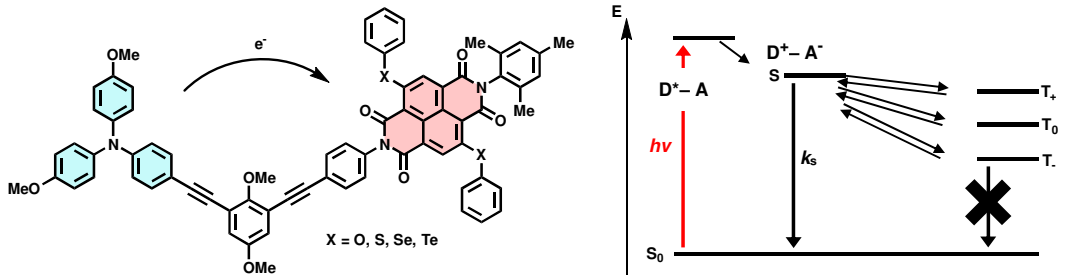

Figure 1: D-A Dyads for investigation of magnetic high field effects (left) and State diagram (right).

Magnetic field dependent measurements revealed significant high field effects increasing in strength from oxygen to the heavier chalcogens (Figure 2). Quantum dynamical simulations were performed to determine whether *g*-tensor anisotropy or Δ*g*-effects are the primary contributor to these findings.

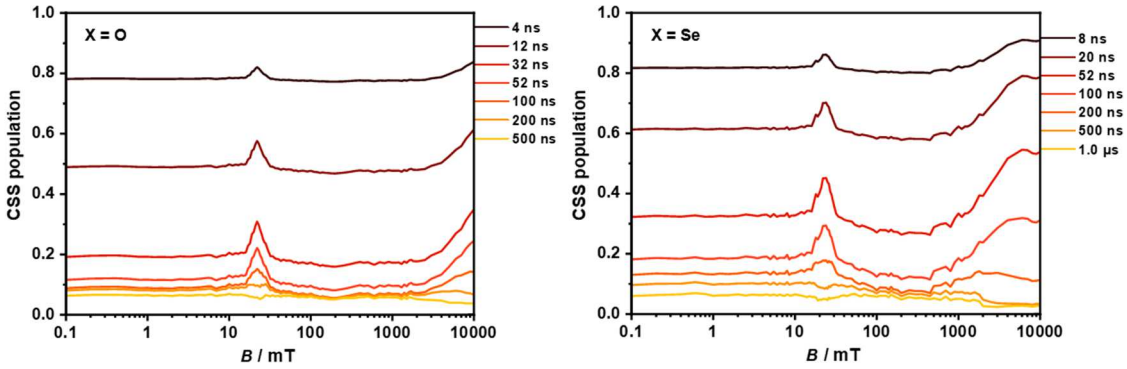

Figure 2: MARY-plot of oxygen (left) and selenium (right) substituted D-A dyads showing magnetic high field effects.

[1] P. Mentzel, L. Gerhards, D. Koppenhöfer, A. Schmiedel, M. Holzapfel, N.N. Lukzen, I.A. Solovyov, U.E. Steiner, C. Lambert, J. Am. Chem. Soc. 2025, 147, 23068-23078.

Poster Abstract

Efficient ^{15}N SABRE Hyperpolarization in Fluorocarbon

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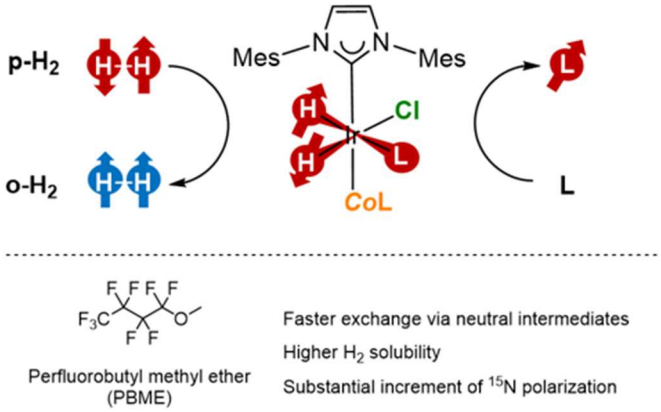
[2]*Centre for Hyperpolarisation in Magnetic Resonance , University of York, Heslington, York, YO10 5DD, UK*

Signal Amplification by Reversible Exchange (SABRE)[1] provides a powerful route to overcome the intrinsically low sensitivity of NMR spectroscopy by transferring spin order from para-hydrogen to target molecules without chemical modification. Here, we investigate perfluorobutyl methyl ether (PBME) [2] as a solvent for SABRE hyperpolarization and ^{15}N detection of nicotine. PBME displays particularly favourable properties for SABRE, combining high hydrogen solubility with efficient catalyst speciation and rapid ligand exchange. Using [IMesIr(COD)Cl] as the precatalyst, nicotine ^{15}N polarization reached 9% with only 1.4 mM iridium. Under optimized conditions, PBME therefore provides approximately 6-12 fold greater ^{15}N polarization per unit of iridium than conventional SABRE solvents such as CD_2Cl_2, $CDCl_3$ and MeOD. The influence of co-ligand identity was subsequently investigated as a strategy to modulate catalyst speciation and substrate exchange, with the aim of achieving a linear dependence of the hyperpolarized response on analyte concentration and thereby exploiting ^{15}N signal amplification for quantitative analytical applications. Depending on the co-ligand, nicotine ^{15}N polarization values of up to 21% were obtained. In addition, the complete immiscibility of PBME with water offers the prospect of combining selective extraction and hyperpolarization within biphasic analytical workflows for complex aqueous samples and biofluids. More broadly, this approach could also be extended to the hyperpolarization of biologically relevant molecules, particularly through the use of fluorinated SABRE catalysts [3] that may enable higher catalyst concentrations in the fluorous phase and thereby further enhance polarization efficiency.



[1] Adams, R. W. et al. Science 2009, 323, 1708–1711
[2] Gater, C. A. et al. J. Phys. Chem. Lett. 2025, 16, 510–517
[3] Floreani, F. et al. Under review at RSC Advances

Poster Abstract

Toward Optical Control of Molecular Spin Qubits: Time-Resolved EPR of Porphyrin-{Cr_7Ni} Assemblies

Giovanna Galuppo[1], Susanna Ciuti[1], Lubomir Loci[1], Selena Lockyer[1], Mor Tsfania[1], Adam Brookfield[1], Alessandro Chiesa[2], Stefano Carretta[2], Eric McInnes[1], Richard Winpenny[1], Alice Bowen[1]

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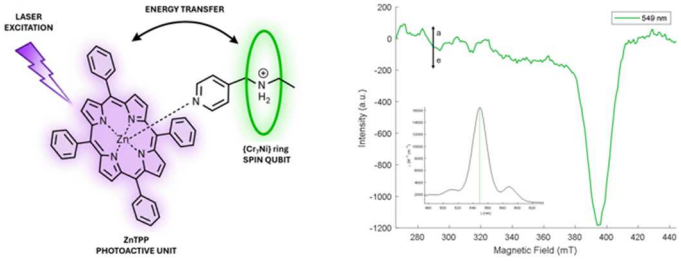
[2] *Università di Parma, Dipartimento di Scienze Matematiche, Fisiche e Informatiche, I-43124 Parma, Italy; Gruppo Collegato di Parma, INFN–Sezione di Milano Bicocca, 43124 Parma, Italy; UdR Parma, INSTM, I-43124 Parma, Italy;*

Molecular spin systems are promising candidates for quantum technologies due to their chemical tunability and well-defined spin states. A key challenge is achieving selective qubit control; light offers a fast and non-invasive approach.[1] Here we investigate hybrid architectures combining zinc tetraphenylporphyrin (ZnTPP) with a {Cr_7Ni} heterometallic ring, a well-established molecular spin qubit platform.[2] We examine how linker length and orientation affect excited-state communication between the chromophore and the spin centre.

Time-resolved electron paramagnetic resonance (trEPR) probes transient spin polarization and triplet dynamics following optical excitation. A clear structure-property relationship emerges, shorter linkers yield stronger coupling, evidenced by suppression of the porphyrin triplet signal and enhancement of ring-centred emission.

These results demonstrate that molecular design tunes spin–photoactive communication and provide insight into transfer pathways, including Förster (FRET) and Dexter (DET) mechanisms, enabling optical control of molecular spin qubits.[3]



(1) Atzori, M.; Sessoli, R. The Second Quantum Revolution: Role and Challenges of Molecular Chemistry. *J. Am. Chem. Soc.* **2019**, *141* (29), 11339–11352. https://doi.org/10.1021/jacs.9b00984.

(2) McInnes, E. J. L.; Timco, G. A.; Whitehead, G. F. S.; Winpenny, R. E. P. Heterometallic Rings: Their Physics and Use as Supramolecular Building Blocks. *Angew. Chem. Int. Ed.* **2015**, *54* (48), 14244–14269. https://doi.org/10.1002/anie.201502730.

(3) Xu, H.; Chen, R.; Sun, Q.; Lai, W.; Su, Q.; Huang, W.; Liu, X. Recent Progress in Metal–Organic Complexes for Optoelectronic Applications. *Chem Soc Rev* **2014**, *43* (10), 3259–3302. https://doi.org/10.1039/C3CS60449G.

Poster Abstract

From π-conjugated to σ-aromatic and aliphatic bridges: Modulating electron transfer and spin chemistry in donor-bridge-acceptor dyads

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[1]*University of Würzburg, Institute of Organic Chemistry, Am Hubland, 97070 Würzburg, Germany*

Bridge engineering is a versatile tool for tailoring properties in donor acceptor compounds. The nature of the bridge – ranging from π-conjugated phenylene groups to aliphatic spacers – plays a decisive role for electronic and exchange coupling within photoexcited biradical states.[1] Carboranes, as third class of linkers, possessing a fundamentally different σ-aromaticity, have shown to promote highly delocalized excited states in mixed-valence systems.[2]

To systematically compare bridge effects, we synthesized isostructural donor-acceptor dyads with *meta*- and *para*-connectivity across aromatic, boron-cluster and aliphatic bridges. Their electron transfer processes and spin chemistry were subsequently investigated using magnetic field-dependant transient absorption spectroscopy and analysed by quantum chemical simulations.

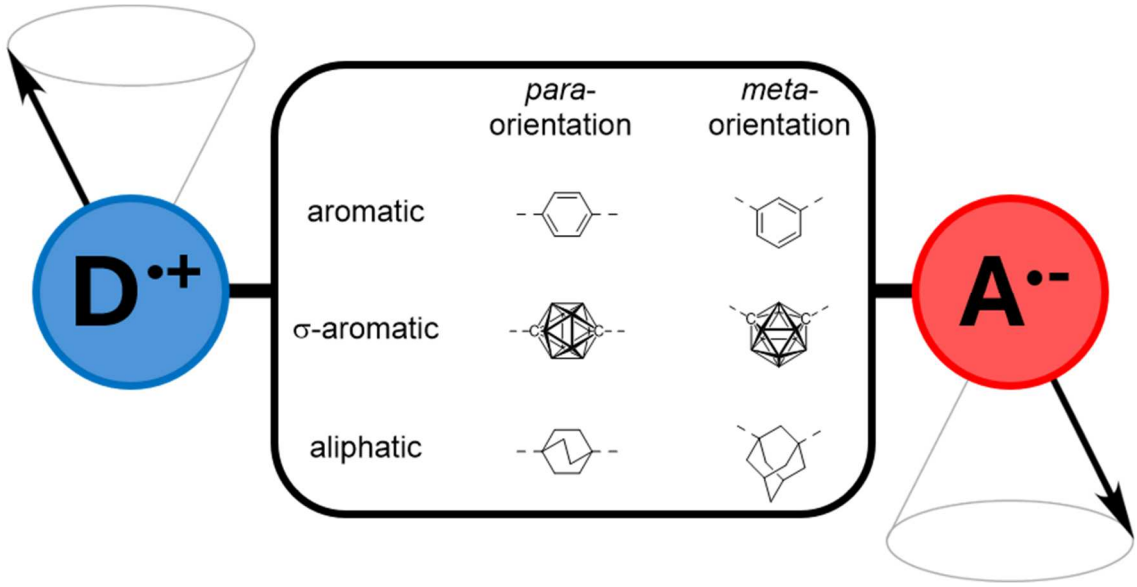

Figure 1: Schematic representation of the investigated donor-acceptor-compounds.

[1] C. Lambert, C. Roger, A. Schmiedel, M. Holzapfel, N. Lukzen, U. E. Steiner, *Phys. Chem. Chem. Phys.*, 2024, **26**, 24983-24994.

[2] L. Wu, X. Zhang, M. Moos, I. Krummenacher, M. Dietz, A. Jayaraman, R. Bertermann, Q. Ye, M. Finze, M. Wenzel, R. Mitric, C. Lambert, H. Braunschweig, L. Ji, *J. Am. Chem. Soc.*, 2024, **146**, 17956-17963.

Poster Abstract

Conditional Enhancement of Radical Pair Dynamics via Chiral State Preparation

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[2]*The Guy Foundation, Beaminster, Dorset, UK*
[3]*School for Data Science and Computational Thinking, Stellenbosch University, Stellenbosch, South Africa*
[4]*National Institute for Theoretical and Computational Sciences (NITheCS),Stellenbosch, South Africa*

Chiral-induced spin selectivity (CISS) has been shown to enhance magnetic sensitivity in radical pair mechanism (RPM) models under specific Hamiltonian conditions, yet whether these enhancements persist across a broader parameter space remains un-tested.

We incorporate the CISS effect as a spin-dependent initial state and recombination operator and systematically evaluate the spin dynamics of a model radical pair across a comprehensive parameter sweep of the RPM Hamiltonian. We characterise the orientational response through symmetric and antisymmetric decomposition of the yield distribution under field reversal, providing a direct quantitative signature of CISS-induced symmetry breaking.

Our analysis demonstrates that CISS does not function as a generic amplifier of mag-netic sensitivity. Claimed enhancements are conditional on the relative alignment of the internal hyperfine and dipolar interaction axes, arising specifically under conditions of non-collinear internal interactions. Extension to a two-nucleus model confirms that these enhancements are sensitive to nuclear spin. CISS-induced effects observed in the single-nucleus model are substantially suppressed when a second collinear nucleus is introduced, with the exception of the hyperfine axis rotation sweep where non-collinear tensor misalignment drives a robust antisymmetric response. These findings indicate that the conditions for CISS-enhanced magnetoreception are more stringent than previously demonstrated, requiring highly ordered and rigid molecular geome-tries to sustain the effect.

[1] Hore & Mouritsen, *Annu. Rev. Biophys.* 45 (2016)
[2] Luo & Hore, *New J. Phys.* 23, 043032 (2021)

Poster Abstract

Spin Relaxation in Pyridyl-Containing Luminescent Triarylmethyl Radicals

Natsuki Hayashi[1], Asato Mizuno[1,2,3], Mizue Asada[4], Toshikazu Nakamura[4,5], Tetsuro Kusamoto[1,2,3,6]

[1]Grad. Sch. of Eng. Sci., The Univ. of Osaka, Toyonaka, Osaka 560-8531, Japan
[2]OTRI-Spin, The Univ. of Osaka, Suita, Osaka 565-0871, Japan
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[4]Institute for Molecular Science, Okazaki, Aichi 444-8585, Japan
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Molecular spin qubits have attracted considerable attention as promising candidates for quantum information processing because their electronic structures and spin properties can be precisely controlled through molecular design. In recent years, open-shell molecular systems based on stable organic radicals have been extensively studied as molecular spin platforms exhibiting excellent spin coherence properties. In particular, luminescent organic radicals are expected to serve as systems capable of spin-state initialization and readout utilizing optical addressability. Such characteristics could enable the realization of "molecular nitrogen-vacancy (NV) centers," in which the optical spin manipulation demonstrated in diamond NV centers is extended to molecular systems. However, studies on the spin coherence properties of luminescent organic radicals remain limited, and clear molecular design guidelines for achieving both excellent optical addressability and long spin coherence times have not yet been established.

In this study, the spin relaxation times of pyridyl-containing luminescent triarylmethyl radicals were investigated by pulsed ESR measurements, focusing on the effects of the number and positions of nitrogen atoms on spin relaxation behavior. In addition, we compared the spin relaxation behavior in frozen solutions and dilute-doped crystals to evaluate the influence of matrix environments. As a result, PyBTM[1] (Fig. 1a) and metaPyBTM[2] (Fig. 1b) in dilute-doped crystal matrices exhibit long T_2 values of approximately 0.5 ms at room temperature (Fig. 1c), which are comparable to those reported for other triarylmethyl radicals. Furthermore, it is revealed that T_1 and T_2 vary depending on the number and positions of nitrogen atoms and the molecular packing, suggesting the possibility of more precise control of spin coherence properties in luminescent triarylmethyl radicals.

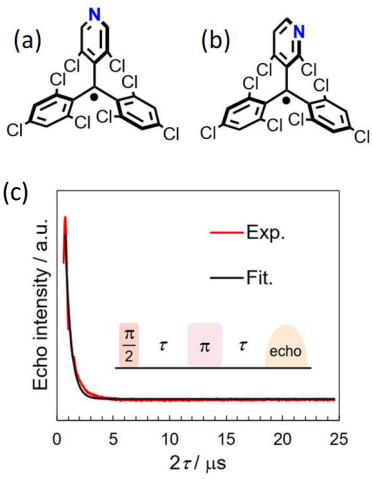

Fig. 1 Chemical structures of (a) PyBTM and (b) metaPyBTM. (c) Hahn echo decay curve of dilute-doped crystals of PyBTM at room temperature.

[1] Y. Hattori, T. Kusamoto, H. Nishihara, *Angew. Chem. Int. Ed.* **2014**, *53*, 11845–11848.
[2] R. Matsuoka, S. Kimura, T. Kusamoto, *ChemPhotoChem* **2021**, *5*, 669–673.

Poster Abstract

A Concealed Non-Kekulé Nanographene as an Addressable Molecular Spin Qubit

Muhammad Imran[1,2], Jan Behrends[3], Xinliang Feng[1,2]

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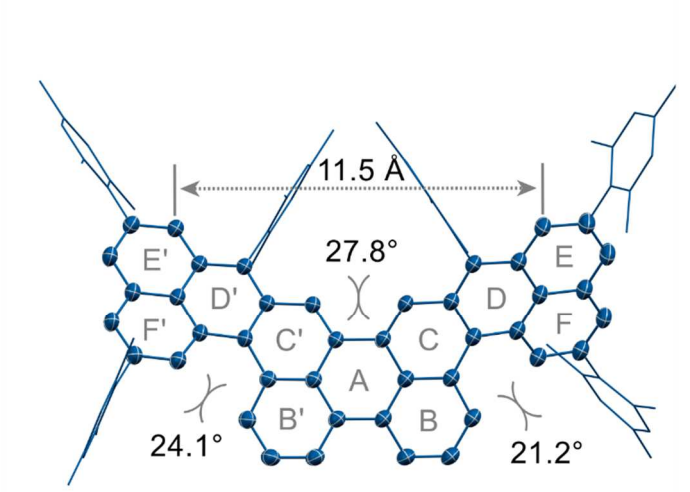
[3]*Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany*

Topological frustration in π-conjugated carbon frameworks offers a powerful route to unconventional concealed non-Kekulé electronic structures and correlated spin states. However, the experimental realization of such systems remains highly challenging because suitable molecular topologies are rare, synthetically demanding, and often insufficiently stable for detailed characterization.

Here, we report the solution-phase synthesis and isolation of a topologically frustrated nanographene with a concealed non-Kekulé structure. A symmetric molecular design, together with kinetic stabilization of the spin-bearing sites, enables crystallization of this otherwise elusive open-shell system, whose structure is confirmed by single-crystal X-ray diffraction. Electron paramagnetic resonance spectroscopy reveals an antiferromagnetically exchange-coupled open-shell singlet ground state with a thermally accessible triplet manifold. Notably, this correlated spin pair displays key features of a molecular qubit platform, including long spin relaxation times and field-selective spin-state addressability. These results provide direct experimental access to spin frustration in a concealed non-Kekulé nanographene and highlight topologically frustrated π-systems as promising metal-free candidates for molecular quantum science.



- *Concealed non-Kekulé topology / Single crystal structure*
- *Field-selective spin-state addressability*
- *Spin qubit behavior / Long T_1 &T_m*

[1] Jiao, T., et. al., *Nat. Chem.* **2025**, 17, 924–932.

Poster Abstract

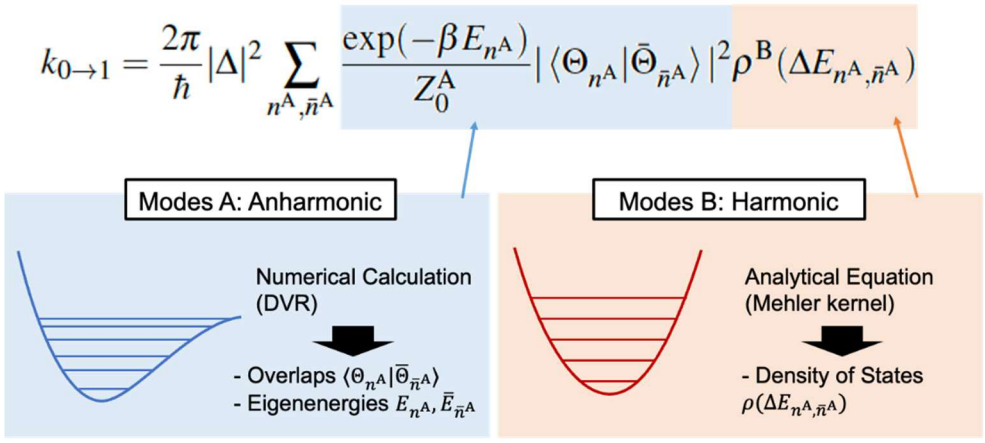
Theoretical Calculation of Fermi's Golden Rule Rate Including the Anharmonicity of Potential Energy Surfaces

Takuma Ito[1,2], Yuki Kurashige[1-3]

[1]*Graduate School of Science, Kyoto University, Japan*
[2]*CREST/*[3]*FOREST, Japan Science and Technology Agency, Japan*

Properties of photofunctional materials are governed by nonadiabatic transitions, and theoretical methods to predict nonadiabatic transition rates are desired. Fermi's golden rule (FGR) combined with the harmonic approximation to the potential energy surface (PES) is one of the most useful approaches to compute rate constants [1,2]. However, the anharmonicity of PES can affect the rate constant by altering energy levels and wavefunctions. Previous studies have investigated the effect of anharmonicity [3-5]. On the other hand, the computational cost of treating anharmonicity in all vibrational modes is high, and methods to incorporate anharmonic effects only for a limited subset of degrees of freedom is desired.

In this study, we propose a method for computing rate constants by dividing vibrational modes into anharmonic modes (set A) and harmonic modes (set B). The rate constant is obtained by combining the numerically evaluated eigenenergies and wavefunction overlaps for modes in A with the density of states for modes in B based on the analytical Mehler kernel. We applied our method to two systems and revealed that the anharmonicity of vibrational modes with high Huang-Rhys factors and high frequencies, or those whose harmonic frequencies are different between initial and final states has an impact on the rate constant.



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Poster Abstract

Upstream Spin-Dependent Modulation of Singlet Oxygen Generation through Radical Pair Dynamics

Yeongcheol Ki[1,2], Seungmin Choi[1,2], Dongcheol Park[1,2], Yeri Son[1], Hyun Gu Kang[1,2], Hyeongyeol Oh[1,2], Won-jin Chung[1], Lewis M. Antill[3*], and Hohjai Lee[1,2*]

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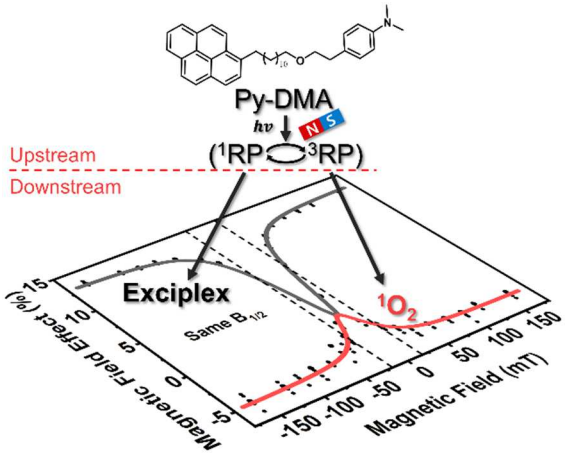
Controlling chemical reactivity through spin dynamics offers a new approach to photochemical regulation, yet magnetic-field sensitivity in oxygen-activation processes has remained difficult to achieve. Here, we demonstrate that singlet oxygen, $O_2(^1\Delta_g)$, generation can be magnetically tuned by decoupling the magnetic-field-sensing step from downstream chemical outcomes. In an exciplex-forming donor-acceptor system, hyperfine-driven singlet–triplet interconversion within a spin-correlated radical pair governs the population of triplet sensitizer states that subsequently generate singlet oxygen [1]. Notably, oxygen does not participate in the spin-sensitive step. Exciplex fluorescence and $O_2(^1\Delta_g)$ phosphorescence act as complementary optical reporters of the singlet- and triplet-derived pathways and exhibit identical magnetic-field dependencies ($B_{1/2}$≈18.4mT), revealing a common spin origin. Time-resolved measurements confirm that magnetic fields modulate $O_2(^1\Delta_g)$ yield without perturbing its decay kinetics, establishing that spin control acts upstream of singlet oxygen generation. These findings introduce a general design principle in which organic radical pair systems function as modular spin-chemical control elements for magnetically tunable singlet oxygen generation, with implications for photodynamic therapy, photocatalysis, and spin-based chemical control.



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Poster Abstract

Hyperpolarisation-Enhanced NMR Spectroscopy of Unaltered Biofluids Using photo-CIDNP

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The direct and unambiguous detection and identification of individual metabolite molecules present in complex biological mixtures constitutes a major challenge in (bio)analytical research. In this context, nuclear magnetic resonance (NMR) spectroscopy has proven to be particularly powerful owing to its ability to provide both qualitative and quantitative atomic-level information on multiple analytes simultaneously in a non-invasive manner. Nevertheless, NMR suffers from a low inherent sensitivity and, moreover, lacks selectivity regarding the number of individual analytes to be studied in a mixture of a myriad of structurally and chemically very different molecules, e.g., metabolites in a biofluid. Here, we describe a method that circumvents these shortcomings via performing selective, photo-chemically induced dynamic nuclear polarization (photo-CIDNP) enhanced NMR spectroscopy on unmodified complex biological mixtures, i.e., human urine and serum, which yields a single, background-free one-dimensional NMR spectrum. In doing this, we demonstrate that photo-CIDNP experiments on unmodified complex mixtures of biological origin are feasible, can be performed straightforwardly in the native aqueous medium at physiological metabolite concentrations, and act as a spectral filter facilitating the analysis of NMR spectra of complex biofluids. Due to its non-invasive nature, the method is fully compatible with state-of-the-art metabolomic protocols providing direct spectroscopic information on a small, carefully selected subset of clinically relevant metabolites. We anticipate that this approach, which, in addition, can be combined with existing high-throughput/high-sensitivity NMR methodology, holds great promise for further in-depth studies and development for use in metabolomics and many other areas of analytical research [1].

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Poster Abstract

Time-resolved EPR spectroscopy of modified cryptochromes

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Cryptochromes are blue-light receptor proteins which react to light excitation by generating spin-correlated radical pairs involving the flavin cofactor and a nearby amino acid residue.[1-5] The radical pair mechanism governs the evolution of these radical pairs, which are initially formed in a distinct spin-correlated singlet spin state.[1,2,6] The coherent interconversion between singlet and triplet spin state is influenced by external magnetic fields which in turn affects the reaction pathways.[7] For this reason, cryptochromes are being discussed as playing a direct role in magnetoreception in migratory birds.[6]

To elucidate the electron spin dynamics of these light-generated spin-correlated radical pairs, time-resolved electron paramagnetic resonance spectroscopy is used. In this work recent spectroscopic data of isotopically enriched, structurally modified cryptochromes with artificial flavin cofactors will be presented.

[1] T. Biskup, E. Schleicher, A. Okafuji, G. Link, K. Hitomi, E.D. Getzoff, S. Weber, Angew. Chem. Int. Ed. 48 (2009) 404-407.
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[3] D. Nohr, S. Franz, R. Rodriguez, L.-O. Essen, S. Weber, E. Schleicher, Biophys. J. 111 (2016) 301-311.
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Poster Abstract

Rationalization of electron spin polarization transfer in chiral porphyrin-[6]helicene-TEMPO triads

Francesco Lazzarin[1], Riccardo Zaramella[1], Roberto Zambon[1], Rajatha Rajendran[2], Yohan Gisbert[2], Jeanne Crassous[2], Barbara Fresch[1], Marilena Di Valentin[1]

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[2]*Institute des Sciences Chimiques de Rennes, CNRS-Université de Rennes 1, Rennes Cedex, France*

Photoexcited triplet states exhibit strong spin hyperpolarisation that can exploited to significantly enhance the sensitivity of EPR techniques, such as light-induced pulsed dipolar spectroscopy, either by using the triplet itself as spin probe or by intramolecular hyperpolarisation transfer to nearby stable radical species.

Previous studies conducted on systems composed of a zinc-porphyrin and a nitroxide covalently linked to a protein scaffold revealed that in the weak-coupling regime this transfer is a consequence of dipolar interactions between the triplet and the radical. Furthermore, flip-flop transitions between the spin levels of the two species were invoked to be responsible for this transfer, with a net spin polarization of the triplet state arising from internal spin dynamics being required to trigger the process [1][2].

With the aim of describing the microscopic interactions, relaxation processes, and coherences involved in this polarisation transfer, a theoretical model based on the density matrix formalism and quantum master equations was developed and exploited to investigate the influence of several physical quantities on the efficiency and magnitude of the transfer. Different coupling strengths between the triplet and the radical were also considered to identify possible polarisation transfer pathways.

The model was tested through comparison between the experimental time-resolved EPR spectra of porphyrin-[6]helicene-TEMPO triads and the simulations of the powder EPR spectra in terms of the calculated spin dynamics. These systems are characterized by a chiral [6]helicene unit as a spacer, whose high racemization barrier fixes the distances between the spin probes in the nm range and enables the investigation of possible chirality effects on the polarisation transfer.

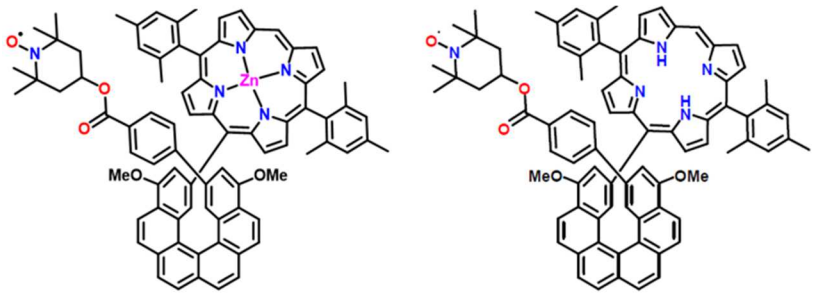

Figure 3 - Structures of the molecular systems investigated in this study

[1] M.G.DalFarra et al. “Electron Spin Polarization Transfer Induced by Triplet-Radical Interactions in the Weakly Coupled Regime”. In: *Phys. Chem. Chem. Phys.* (2020).

[2] D. Panariti et al. “Long-lived light-induced electron spin polarization in porphyrin triplet states and the dynamic Jahn–Teller effect”. In*: J. Chem. Phys*. 162 (2025), pp. 114201, 1–12.

Poster Abstract

Exploring Porphyrin Triads as Molecular Compasses

Sam A. Leggatt[1], Deepannita Samanta[1], Gabriel Moise[1], Damyan Frantzov[1], Christiane R. Timmel[1], Harry L. Anderson[1]

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The coherent evolution of spin-correlated radical pairs can be exploited to detect Earth-strength (50 μT) magnetic fields. [1] The proposed radical pair mechanism, which is a leading hypothesis for avian magnetoreception, is being explored in chemically tunable molecular compasses. While magnetic field effects have been reported in several synthetic molecular compounds, only one system has previously shown sensitivity to the strength and orientation of an Earth-strength magnetic field. [2] In this compound, the strength and readout of the magnetic field effect limit its applicability as a sensor.

This project involves the design, synthesis and spectroscopic characterisation of new donor–porphyrin–acceptor molecular triads with Earth-strength magnetic field effects, intending to develop structure-property relationships for molecular compass design. Inspired by the work of Poddutoori, van der Est *et al.* [3], we have initially targeted modular approaches to porphyrin triad assembly. An aluminium porphyrin triad was prepared by self-assembly in solution. Fluorescence quenching and ns-TA reveal the formation of a radical pair, but its lifetime (< 1 ns) is too short for magnetic field effects. Consistent with the short lifetime, the radical pair was not observed by transient EPR; instead, the EPR spectra revealed that the electron donor influences triplet spin polarisation. These results demonstrate the value of modular synthesis for evaluating molecular compass candidates.

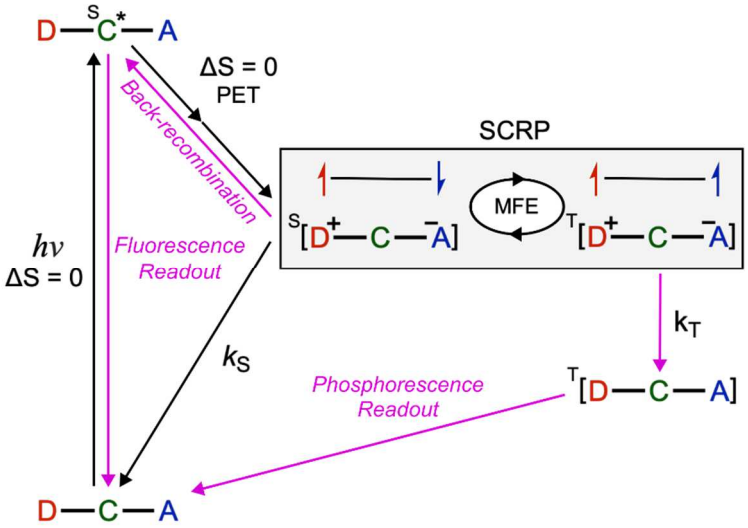

Figure 1. Schematic for the radical pair mechanism in a donor-chromophore-acceptor (D-C-A) compound. The spin-correlated radical pair (SCRP) is generated following photoinduced electron transfer (PET). The evolution of the SCRP exhibits a magnetic field effect (MFE) which is optically detectable (shown in pink).

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Poster Abstract

Insights into the structure–property relationships governing magnetoluminescence in Non-Kekulé triarylmethyl diradicals

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Organic diradicals exhibiting magnetoluminescence (ML) have attracted significant attention for molecular spin–optical manipulation. In recent years, five non-Kekulé triarylmethyl-based diradicals have been reported to display ground-state (GS) modulated ML at the molecular level [1–2]. Two of these diradicals show distinct emission wavelengths for triplet (~650 nm) and singlet (~720 nm) excitons, with GS populations tunable by an external magnetic field at low temperatures [1]. In contrast, three other diradicals exhibit ML without a distinct singlet exciton emission band, showing instead modulation of overall photoluminescence intensity around ~650 nm [2]. These differences raise fundamental questions about the origin of singlet/triplet exciton emissions and the influence of molecular structure on ML response.

Here, we employ quantum chemistry methods to investigate the ML behavior of diradicals **1a** and **2a** (Figure 1). Our results indicate that, in both systems, the low-lying triplet and singlet excitons correspond predominantly to local and radical-to-radical charge-transfer (CT) states, respectively. However, subtle differences in their deactivation pathways explain their distinct ML properties. In diradical **2a**, the CT character of the singlet exciton induces a significant conformational change that destabilizes the ground state, reducing the emission gap and leading to a red-shifted, non-radiative near-infrared emission. In contrast, diradical **1a** undergoes a smaller structural distortion, resulting in a weakly emissive singlet exciton at ~720 nm. These findings provide design guidelines for tuning ML properties in non-Kekulé diradicals.

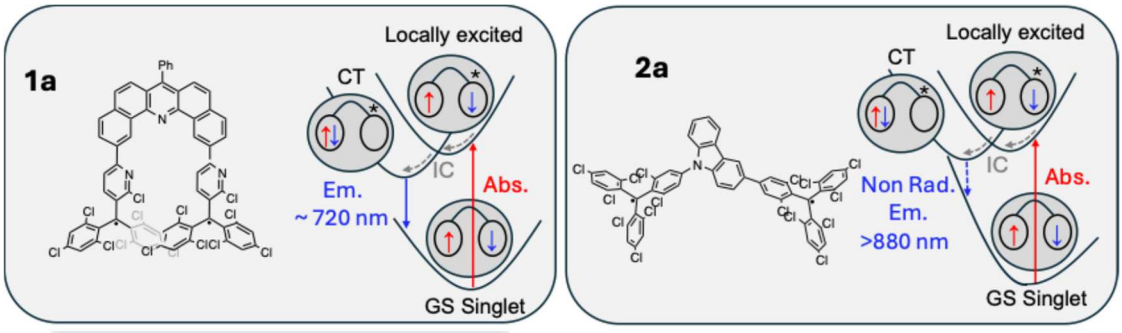

Figure 1. Molecular structure of diradicals **1a** and **2a,** each with a schematic representation of the potential energy deactivation pathway of the singlet upon excitation.

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[2] Abdurahman et al. *Light Sci. Appl*. **2023**, 12, 272; b) Mizuno et al. *J. Am. Chem. Soc.* **2024**, 146, 18470; c) Wang et al. *Angew. Chem., Int. Ed.* **2025**, 64, e202513593

Poster Abstract

Selective Observation of Radical Pair Spin Dynamics Using Pump–Push Spectroscopy

Yoshitoshi Matsushita[1], Akihiro Tateno[1], Kiminori Maeda[1], Ulrich. E. Steiner[2], Christoph Lambert[3]

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[2] *University of Konstanz*
[3] *University of Würzburg*

Photochemical reactions proceed via radical pairs (RPs), which preserve the spin multiplicity of their precursor. For example, an RP generated from a singlet (S) excited state initially occupies an S state; however, this does not correspond to an energy eigenstate of the RP, but rather to a linear superposition of eigenstates, referred to as coherence. As a result, when the RP state is described in the singlet (S)–triplet (T) basis, coherent S–T mixing arises. Direct time-resolved observation of this S–T mixing is challenging. Lambert et al. employed pump–push spectroscopy based on two-step photoexcitation to observe coherent dynamics known as spin quantum beats [1]. When discussing the relationship between magnetic field effects and coherent dynamics, it is important to determine the extent to which a quasi-steady state depends on the magnetic field once the radical pair spin system reaches that state via decoherence or relaxation. In this context, the situation becomes even more complex when transient absorption from multiple species overlap.

Therefore, in this study, we used the 685 nm as the probe wavelength, which selectively monitors the radical pair (RP), while applying a push pulse at 650 nm. The effect of the push pulse on the transient absorption signal was then evaluated. Letting (f) denote the fraction of RPs excited by the push pulse, the following expressions are obtained:

TA signal without push pulse: $\Delta A(t\,, B) = \varepsilon_{RP}^{685\ \mathrm{nm}}[RP]_t^B$ (1)

TA signal just after a push pulse: $\Delta A(t_p\,, B) = \{1 - f(0.24P_S + P_T)\}\varepsilon_{RP}^{685\ \mathrm{nm}}[RP]_t^B$ (2)

Effect (2)/(1)-1: $Eff = \frac{\Delta\Delta A(t_p\,,B)}{\Delta A_{no-push}(t_p\,,B)} = -f(0.24P_S + P_T)$ (3)

By this we could obtain the pure S-T mixing dynamics except the factor *f.*
Furthermore, time evolution of the T_+ and T_- spin stats were examined using Magnetic Field Switching Experiments (SEMF method). By combining experiment and simulation, we are trying to identify the origin of the low-field effect.

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Poster Abstract

Predicting Electron Spin Relaxation Rates of Triplet Chromophores from Molecular Dynamics

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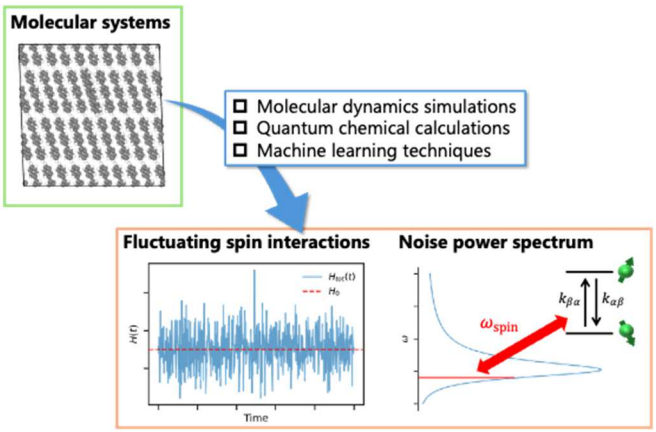
Photoexcited organic chromophores can generate transient spin polarization through sublevel-selective intersystem crossing, enabling applications in dynamic nuclear polarization [1], masers [2], and quantum sensing based on ODMR measurements [3,4], all at room temperature. Understanding the microscopic mechanism of electron spin relaxation in such molecular spin systems is essential for designing long-lived qubits and optimizing host-guest environments. Previously, we investigated electron spin-lattice relaxation rates in pentacene doped into *p*-terphenyl crystals using Redfield theory combined with a harmonic oscillator model and quantum chemical calculations [5]. Although the calculated relaxation rates qualitatively reproduced experimental trends, the fluctuations of zero-field splittings (ZFS) were treated within the linear vibronic coupling (LVC) approximation, limiting the quantitative description of complex host-guest fluctuations in molecular crystals.

In this work, we go beyond the harmonic and LVC approximations by combining molecular dynamics (MD) simulations with multireference electronic-structure methods and machine learning techniques. Using MD simulations and machine learning predictions of ZFS tensors with GPU acceleration, we evaluated ZFS fluctuations along trajectories consisting of more than ten million time steps. The present framework provides a scalable route toward quantitative prediction of electron spin relaxation rates in condensed-phase molecular spin systems.



[1] A. Henstra, W. Wenckebach *et al.*, *Phys. Lett. A* **1988**, *134*, 134.
[2] M. Oxborrow, N. M. Alford *et al.*, *Nature* **2012**, *488*, 353.
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[5] K. Miyokawa, and Y. Kurashige, *Phys. Chem. Chem. Phys.* **2026**, *28*, 1230.

Poster Abstract

The Semiquinone as a Distinct Structural State in the *Erithacus rubecula* Cryptochrome 4a Photocycle

Monika Kish[1,3], Suchitra Pradha[1,2,4], Jessica L. Ramsay[1,2,5], Paloma Munguía Salazar[1,2], Jonathan Phillips[1,3,6], and Daniel R. Kattnig[1,2]

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[4] *Current affiliation: Bristol Veterinary School, University of Bristol, Bristol, United Kingdom.*
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Cryptochromes are flavoproteins proposed to act as light-dependent sensors of the Earth's magnetic field in migratory species. In the European robin (*Erithacus rubecula*), the cryptochrome isoform 4a (ErCry4a) goes through a photocycle that involves oxidized, semiquinone, and reduced states, with the semiquinone state generating the radical pair, which previously has been proposed as the quantum mechanism behind avian magnetoreception.

Using Hydrogen–Deuterium Exchange Mass Spectrometry (HDX-MS), we show that ErCry4a undergoes specific redox-dependent structural changes connecting light-induced photochemistry to large-scale protein motions. We identify key conformational shifts in several structural regions, including the PBL, PL, α17 helix, and α22/α23 network. Importantly, the semiquinone state emerges as a distinct, biologically active signaling form rather than a simple intermediate. Unlike the fully reduced state, which becomes more rigid, the semiquinone exhibits transient destabilization of critical regions, supporting its proposed role as a signaling state. The distal region of the C-terminal tail remains highly flexible across states.

Together, these findings provide new insight into how cryptochrome may translate quantum photochemical events into molecular signals required for avian navigation.

[1] Kish, M., Pradhan, S., Ramsay, J. L., Munguía Salazar, P., Phillips, J., & Kattnig, D. R. (2026). *Distinct structural dynamics of the semiquinone state define a signalling pathway in avian cryptochrome*. arXiv. https://doi.org/10.48550/arXiv.2604.19579

Poster Abstract

Exploring the Sensitivity Limits of Nanodiamond Quantum Sensors for Biomedical Applications

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[2]*Department of Physics, Warwick University, Warwick*

The nitrogen-vacancy (NV) centre in diamond is an optically addressable spin defect widely used in quantum sensing. A key area of development in recent years is the use of NV-doped nanodiamonds (NDs) in biomedical applications such as diagnostics and screening.[1] NDs are promising sensors since they are chemically inert and biocompatible whilst exhibiting stable, non-bleaching fluorescence with emission extending into the biological optical window, enabling fluorescence imaging in living systems.[2]

Of particular interest is their potential for intracellular free-radical detection, as free radicals are indicators of oxidative stress associated with numerous diseases.[3] However, while intracellular free-radical detection using NDs has been demonstrated,[4] relatively little is known about the fundamental sensitivity limits of these sensors and how various engineered or intrinsic ND properties influence the achievable sensitivity. Here we develop a quantitative framework based on experimentally validated T_1 time modelling and Fisher information analysis to investigate how factors such as NV spin relaxation, nanodiamond geometry, NV concentration and adsorption processes influence the minimum detectable free-radical concentration.

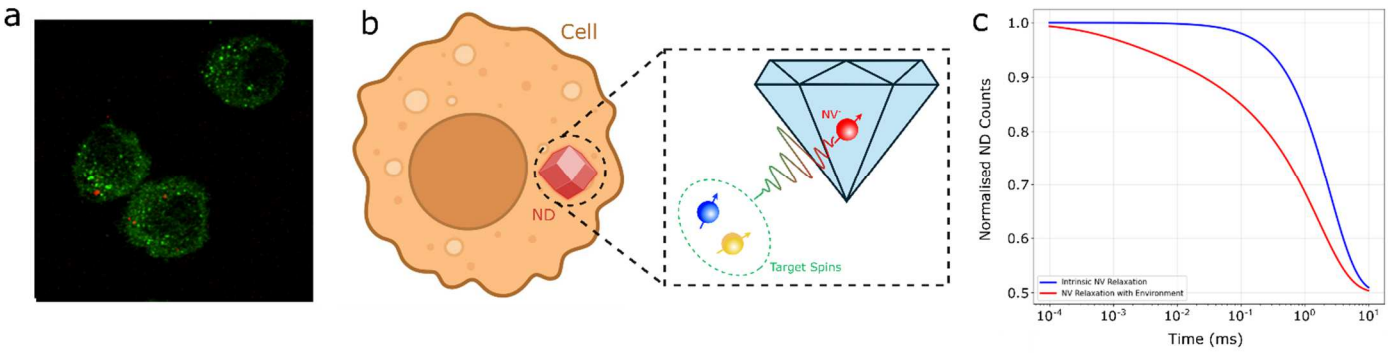

Figure 2 a) A calcium image of cells containing NDs (red dots).b) Schematic of a ND within a cell where an NV centre is coupled to intracellular spins. c) T_1 relaxometry simulation of a ND in the absence (blue line) and presence (red line) of free radicals. Dipolar coupling between the NV centres and tumbling free radicals leads to a drop in the observable ND T_1 time.

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[2] *ACS Nano* **2021**, 15, 12869−12879.
[3] *Cell Death Discov.* **2025,** 11, 19.
[4] *APL Mater.* **2023,** 11, 090603-2.

Poster Abstract

Magnetic-Field Effects in Photo-CIDNP of Flavin-Tryptophan Dyads

Guzel Musabirova[1], Olga B. Morozova[2], Alexey S. Kiryutin[2], Ivan V. Zhukov[2], Tobias Theiss[3], Tanja Gulder[3], Alexandra V. Yurkovskaya[2], Jörg Matysik[1]

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[2] International Tomography Center, SB RAS, Russia
[3] Leipzig University, Organic Chemistry, Germany

Photochemically induced dynamic nuclear polarization (photo-CIDNP) is a sensitive NMR approach for studying light-induced radical-pair reactions and the spin dynamics that control nuclear hyperpolarization [1,2]. In flexible donor-acceptor systems, however, conformational heterogeneity can strongly affect the balance between different polarization pathways. Here, we investigate this effect in flavin-tryptophan dyads connected by oligoproline linkers [3].

Using field-cycling ^{1}H photo-CIDNP NMR, the magnetic-field dependence of nuclear polarization was measured from 1 mT to 9.4 T. The high-field CIDNP patterns were mainly consistent with Δg-driven polarization caused by intermolecular radical encoun-ters [4]. In contrast, short oligoproline dyads showed pronounced low-field and intermedi-ate-field features. These signals were strongest for minor conformers and displayed uni-form emissive polarization, indicating J-resonance CIDNP formed through intramolecu-lar biradical recombination [4].

The data show that proline cis-trans isomerization controls the spin-selective reactivity of the dyads [4]. Minor cis-containing conformers bring the flavin and tryptophan units into compact geometries, increase the exchange interaction, and enable intramolecular biradical pathways. The dominant trans-rich conformers, especially in longer linkers, favor intermolecular processes and therefore produce mainly Δg-type polarization. Time-resolved photo-CIDNP measurements further support this separation of intra- and in-termolecular mechanisms.

Overall, field-cycling photo-CIDNP reveals how small conformational subensembles can dominate spin-dependent reactivity, even when they represent only a minor fraction of the molecular ensemble. This makes magnetic-field-dependent photo-CIDNP a powerful tool for detecting transient biradical states and for understanding structure-spin dynamics relationships in flexible photoactive donor-acceptor systems.

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[4] Musabirova, G. et al. *J. Am. Chem. Soc.* **2026**, 148, 15897–15910.

Poster Abstract

Open-Shell Carbene-Metal-Amide Emitter for Intramolecular Triplet–Doublet Interactions

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Carbene-metal-amide (CMA) complexes are organometallic emitters that can efficiently generate triplet excited states through rapid intersystem crossing promoted by metal centre-derived spin-orbit coupling. Recent studies have shown that triplet excitons generated in CMA-based organometallic hosts can be efficiently transferred to organic radical emitters through triplet-to-doublet energy transfer [1]. This process provides a promising strategy for harvesting normally dark triplet excitons without relying on conventional singlet–triplet spin-flip pathways. However, these systems have mainly been investigated in intermolecular host–guest blends, where the distance, orientation, and electronic coupling between the triplet donor and radical acceptor are difficult to control.

In this study, we investigate an intramolecular triplet-doublet system based on a CMA radical, in which a triplet-generating CMA chromophore and a stable organic radical are incorporated within a single molecular framework. By covalently linking the CMA unit to a radical spin centre, this molecular design provides a structurally defined platform for studying intramolecular triplet–doublet interactions and exciton dynamics. We examine how the radical spin may influence intersystem crossing and spin-forbidden optical transitions of the CMA chromophore, as well as spin-state evolution potentially involving doublet and quartet radical–triplet pair states. Establishing such an intramolecular triplet–doublet system is expected to provide fundamental insight into exciton coupling in open-shell molecular systems and guide the development of optically addressable photomagnetic systems.

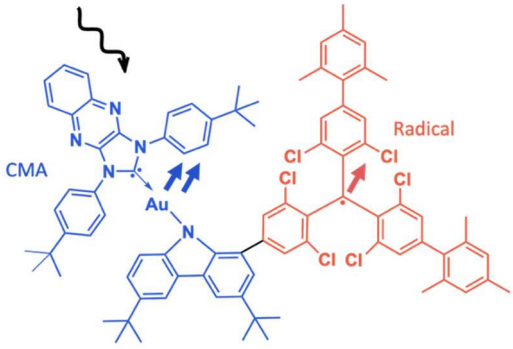

Figure 1. Molecular design of the CMA radical system.

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Poster Abstract

The effect of isotopic substitution on magnetic field effects in avian cryptochromes

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Some night-migratory songbirds possess a magnetic sense that provides directional cues during migration [1]. This sense requires short-wavelength visible light, supporting a hypothesis based on the photogenerated spin-correlated radical pairs including flavin adenine dinucleotide (FAD) [2]. The proposed magnetoreceptor is the cryptochrome-4 flavoprotein found in avian retinal cells. Electronic excitation of FAD leads to an electron transfer cascade along a chain of four tryptophan residues generating the spatially separated radical pair necessary for a magnetic field effect (MFE) [3] which arises from the different magnetic environments of each radical.

Here, we present initial results of a key test of the radical pair mechanism in cryptochromes, namely that nuclear hyperfine interactions should have an effect on the magnetosensitivity. Broadband cavity-enhanced absorption spectroscopy has been applied to compare MFEs in mutated robin cryptochromes with both naturally occurring and ^{13}C enriched flavins. The magnetic response is found to be significantly different with the characteristic $B_{1/2}$ increasing by 30% upon isotopic labelling.

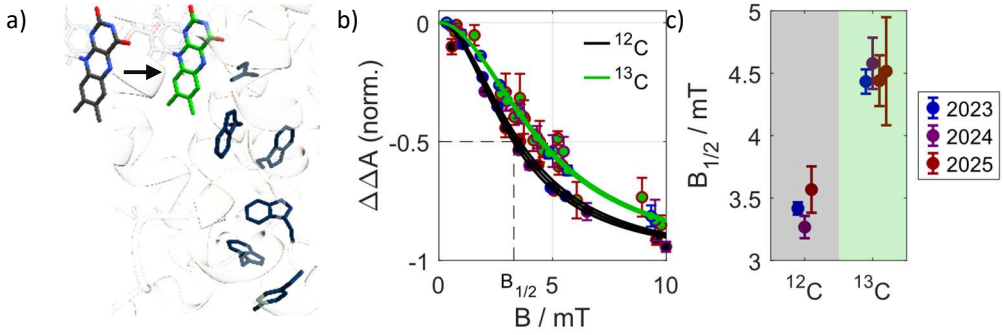

Figure 4: (a) Within the cryptochrome, carbon atoms in FAD are substituted for ^{13}C (green). (b) Magnetic sensitivity of reaction yields in substituted and unsubstituted systems. (c) Comparison of fitted $B_{1/2}$ values; error bars represent one standard error.

Ongoing behavioural studies will now test this effect on birds fed a diet including ^{13}C enriched flavin. A change in navigational behaviour in these birds would strongly support the involvement of FAD-containing radical pairs in this magnetic sense [4].

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Poster Abstract

Mechanistic analysis of MagLOV toward its application as a protein-based quantum sensor

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Measuring intracellular temperature, pH, and magnetic fields at microscopic spatial scales is essential for understanding biological phenomena from a physicochemical perspective. Quantum sensing has emerged as a promising approach for achieving such measurements, and a wide variety of sensors and methodologies have been actively investigated. In recent years, protein-based quantum sensors utilizing the spin states of photochemically generated radical pairs (chemical intermediates composed of two radicals) have gained considerable attention. Several fluorescent proteins that form radical pairs exhibit magnetic-field-dependent changes in fluorescence intensity [1], and active efforts are underway to exploit this phenomenon for biological sensing applications [2]. These sensors can be genetically encoded, allowing intracellular expression and facile fusion with target molecules for precise localization [3].

MagLOV, the focus of this study, is a protein engineered through random mutagenesis and screening to maximize magnetic-field-induced changes in fluorescence intensity. The magnetic field effect is believed to originate from the formation of radical pairs. While conventional radical-pair-based magnetic field effects detected via fluorescence intensity were typically below ±5%, MagLOV exhibits an exceptionally large effect of approximately −40% in *Escherichia coli* cells [1]. Owing to this remarkable property, MagLOV has been regarded as a promising candidate for protein-based quantum sensors. Optically detected magnetic resonance (ODMR), as well as functional modifications, has already been demonstrated [2].

However, the fundamental reaction mechanism underlying this phenomenon remains poorly understood, and rational guidelines for improving sensing performance and molecular engineering have yet to be established. In this presentation, we report the results of mechanistic analyses using fluorescence and transient absorption measurements. We further discuss the challenges and future prospects of MagLOV for quantum sensing applications.

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Poster Abstract

Revisiting Electron-Electron Dipolar Interactions in Geminate Radical Pairs: An Approach Based on the Stochastic Liouville Equation

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The radical pair mechanism (RPM) is the central mechanism of spin chemistry, describing how spin-correlated radical pairs with spin-selective recombination reactions can develop sensitivity to weak magnetic fields [1]. The overwhelming majority of these reactions occur in solution, such that the radicals are free to diffuse. This motion modulates the action of the electron-electron dipolar (EED) interaction, which is thought to impose significant spin relaxation. While this effect has been acknowledged right from the mechanism's discovery [2,3], it has rarely been included in theoretical models, because of the difficulty of coupling coherent spin evolution to spatial mobility in 3D, which is required to fully capture the effect. Only a single study has attempted to accommodate EED interactions in diffusing radical pairs but was limited to a Monte Carlo approach with a single-nucleus radical pair [4]. The resulting data is sparsely sampled and noisy, leaving gaps in the interpretability of EED interactions in the RPM to date.

We revisit this problem using the stochastic Liouville equation, which carries none of the sampling noise that plagued that previous study. The radicals' radial separation is accounted for using a finite-difference basis in a transformed radial variable [5]; a spherical harmonic basis is used to model that angular dependency. Together, this provides a comprehensive description of diffusive radical pairs subject to distance-dependent reactivity and general inter-radical interactions, including directional EED interactions. We employ this model for a two-proton RP, systematically varying the recombination rate constant and the diffusion coefficient. We observe that the high-field effect can be enhanced by the EED interaction. In contrast, the low-field effect is greatly suppressed, particularly in highly viscous solvents. Notably, unlike predicted in [4], the canonical form and orientation of the magnetic field effect is preserved in all calculations. These findings illuminate the fundamental action of the EED interaction, informing future studies in viscous environments, including radical pair reactions in biological systems.

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Poster Abstract

CW-EPR applied to Heritage Science: insights into the degradation mechanism of celluloid

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Celluloid (cellulose nitrate with camphor as plasticiser) was the very first plastic to be successfully introduced in the market and is probably one of the most problematic materials of the contemporary era in terms of conservation. Entailing strong yellowing, embrittlement and extensive cracking, the severe alteration of celluloid objects in museums and archives is nowadays causing the loss of a significant part of cultural heritage. Not only is the degradation of such a material autocatalytic, but it is also hazardous for nearby objects due to the nitrogen oxides released in the process [1]. Crucial is the research on the degradation pathways to understand how to mitigate them and so preserve both celluloid and proximate materials. While the mechanism hypotheses proposed in the literature rely on the identification of reaction products alone [2], the present work introduces new insights on the radical reactions involved thanks to the use of CW-EPR measurements. These were performed on mock-up samples artificially aged in a climatic chamber for different durations, as well as on naturally aged objects from the Deutsches Museum of Munich (Germany). A series of analyses in X-band allowed to study the formation or radicals in celluloid during the exposure to light and their decay occurring in the following dark storage. Such investigations were combined with ATR-FTIR and colourimetric analyses, which helped detecting the effects of radical quenching in the material. Q-band EPR analyses were implemented to better characterise the detected radicals, which were hypothesised to be of nitroxide type. Even though similar radicals were found in UV-irradiated cellulose nitrate by Yamauchi et al. in 1993 [3], such species have never been included in the mechanism for celluloid degradation, to the authors' knowledge. Finally, EPR analyses on aged cellulose nitrate and celluloid films with different amounts of camphor suggested the plasticiser might have a role in the radical process.

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Poster Abstract

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 coupling and 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 couplings and substitution positions for an optimised molecular design.

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Poster Abstract

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.

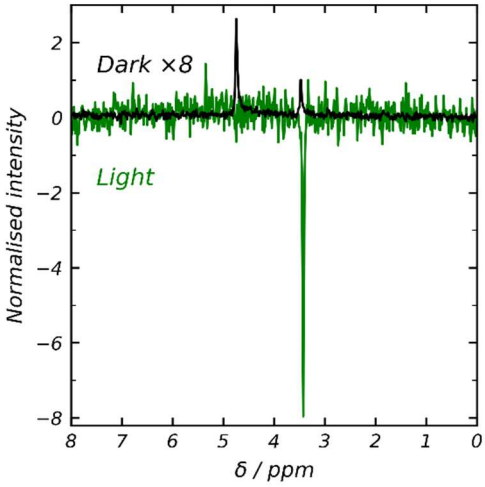

Figure 1: ^{1}H NMR enhancement of glycine using the RTPM: illumination shows 8×DNP gain over 8 dark scans.

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Poster Abstract

EPR study of mononuclear iron centers in ISCA1 related to magnetic field response

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The iron-sulfur (Fe-S) cluster assembly homolog 1 (ISCA1) is a ubiquitous protein involved in the biosynthesis of Fe-S clusters and conserved in various organisms. ISCA1 binds to [2Fe-2S], [3Fe-4S] clusters [1]. Also, recent studies have reported that ISCA1 bind to mononuclear iron [2]. Previous work has shown that pigeon ISCA1 (clISCA1), human ISCA1 (hsISCA1), and fly ISCA1 (dmISCA1) undergo structural changes in the mononuclear iron-bound state in response to magnetic fields [3,4]. When Fe was removed, the magnetic field effect disappeared. So, electron spin of irons (Fe, Fe-S clusters) may play an important role for magnetic responsibility.

In this study, we aimed to clarify the electronic state of the mononuclear iron center bound to ISCA1. For this purpose, we conducted electron paramagnetic resonance (EPR) measurements of ISCA1 from *Columba livia* (clISCA1), *Homo sapiens* (hsISCA1), *Erithacus rubecula* (erISCA1), and *Drosophila melanogaster* (dmISCA1) (UniProtKB accessions: P0DN75, Q9BUE6, A0A7K7H5B4, and Q8T3X9), and compared the results among these species. As a result, a rhombic EPR signal at g = 4.3 and split signals (g = 4.38 and 4.13) were observed in clISCA1 and erISCA1 (Figure 1). This result indicates that ISCA1s have at least two Fe-binding sites with different ligand fields. On the other hand, no EPR signal at g = 4.3 was observed in hsISCA1, and no split signals (g = 4.38 and 4.13) were observed in dmISCA1 (Figure 1). Also, the ISCA1s do not contain Fe-S clusters but iron in all species. This result suggests that the main magnetic center contributing to the magnetic field response may be mononuclear iron.

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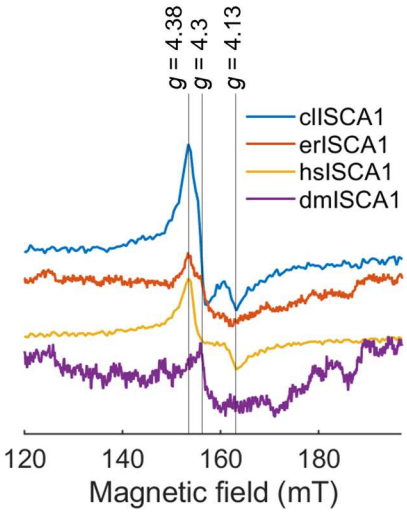

Figure 1. EPR spectra of 7 mg/mL clISCA1, erISCA1, hsISCA1, and dmISCA1.

Poster Abstract

Small Singlet-Triplet Gaps: A Multireference Electronic Structure Study using Trimethylenemethane-Type Biradicals as Model Systems

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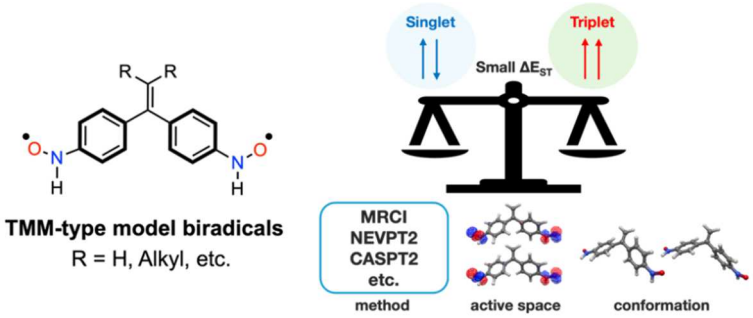
Organic biradicals provide a sensitive platform for examining how molecular topology, spin delocalization, and electron correlation control the energy ordering of low-lying spin states [1,2]. Molecules with small singlet-triplet (S-T) gaps occupy a delicate energetic regime in which modest structural or electronic perturbations can substantially alter the relative stability of the lowest singlet and triplet states. Accurate theoretical prediction of such gaps remains nontrivial, because the relevant spin states may involve different degrees of static and dynamic correlation, and small absolute errors in total energies can translate directly into qualitatively incorrect spin-state energetics [1-4]. In particular, low-lying singlet states in organic biradicals often possess pronounced multiconfigurational character. Although complete-active-space (CAS) wavefunctions provide a natural starting point for describing this static correlation, quantitative S-T gaps also require an appropriate treatment of dynamic correlation [3,4].

In this study, we used trimethylenemethane-type (TMM-type) biradicals as model systems to obtain reliable theoretical estimates of small S-T gaps. These molecules are well suited for this purpose because their exchange interactions have been shown experimentally to depend sensitively on molecular structure, conformation, and spin-density distribution [5,6]. We calculated their S-T gaps using multireference dynamical correlation methods, including NEVPT2, CASPT2, and MRCI, based on CASSCF reference wavefunctions, and examined the dependence of the resulting spin-state energetics on the electronic-structure method, active-space selection, and molecular geometry. These comparisons reveal the sensitivity of small S-T gaps to both methodological and structural choices, and highlight the importance of post-CASSCF multireference treatments for reliable evaluation of such gaps.



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Poster Abstract

Bridge conjugation towards control of spin multiplicity in mesitylated trityl biradicals

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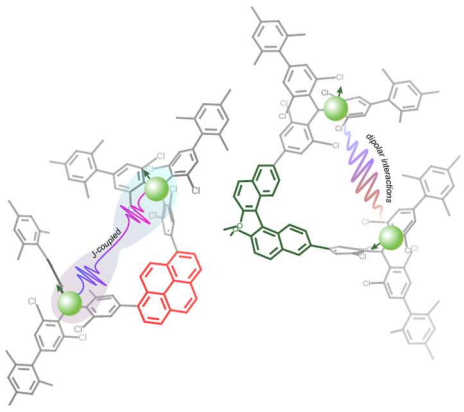
Molecular spin qubits present a promising frontier for quantum information science [1], with the possibility for extended spin lifetime and spin-optical readout.[2] Organic biradicals are compelling spin-qubit candidates owing to their scalable fabrication, precise control over spin placement and promising magnetic properties. A critical strategy for modulating spin-qubit properties varies the bridging unit connecting the two radical centres [2]. We report the design and development of a pair of trityl-based biradicals with similar interspin distance, but where linking of radical centres with chiral (BinOMe) and achiral (Pyrene) bridges enables control of overall spin multiplicity of paramagnetic species via π-conjugation.

Temperature-dependent continuous-wave EPR measurements were employed to probe the ground-state spin character, while pulsed EPR techniques, including inversion recovery, Hahn echo and Rabi nutation experiments, enabled the investigation of spin-relaxation and coherent spin manipulation. SQUID magnetometry revealed the magnetic profile of the spin interactions within the biradical moiety. Complementary Density Functional Theory and EPR simulations supported the experimental findings and provided robust estimates of spin–spin coupling parameters. The chiral system displays EPR and SQUID magnetometry signatures of a weakly coupled biradical, whereas the achiral system presents as a strongly coupled system with a thermally accessible triplet state. Rabi nutations reveal unusual coupling behavior in the chiral system; asymmetric oscillations indicate microwave-driven spin transitions within a thermally populated triplet manifold. These results provide critical insights into the design rules for next-generation molecular qubit architectures.



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Poster Abstract

EPR Characterization of Peroxy Radicals in Industrially Irradiated PTFE

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Polytetrafluoroethylene (PTFE) owes its widespread industrial success to its outstanding chemical inertness, thermal stability and low friction. An industrially relevant class of PTFE products — micronized PTFE powders, ubiquitous as additives in inks, other plastics, lubricants and electronics — is obtained by exposing the polymer to high-energy irradiation to reduce its molecular weight [1]. This process, however, generates perfluoroalkyl radicals that, in the presence of oxygen, evolve into peroxy radicals and ultimately into species such as perfluorooctanoic acid (PFOA) [2], a persistent and toxic compound whose presence in materials has recently been heavily restricted by the European Union [3]. Understanding how processing conditions govern the formation and fate of these radicals is therefore a pressing issue for the industrial production of PTFE micropowders, at the interface of polymer chemistry and environmental regulation.

EPR spectroscopy is the method of choice to detect and characterize these radicals [2,4], yet little is known about PTFE micropowders from real industrial processes and how process parameters affect radical formation. Here we combine a detailed spectroscopic characterization of the radicals — via continuous-wave (CW) EPR at variable temperature, spectral simulation, and complementary pulsed EPR experiments (ESEEM/ENDOR) — with a quantification of how industrial preparation and irradiation conditions govern their formation in PTFE micropowders.

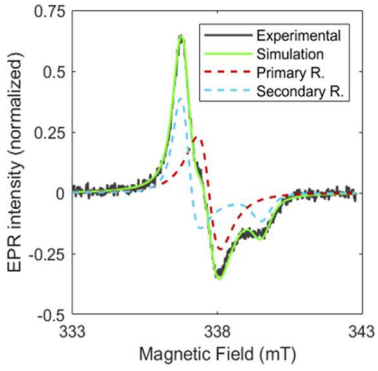

Figure 1. CW-EPR spectrum of irradiated PTFE and simulation

Simulation of the CW spectra (Fig. 1) allowed us to semiquantitatively track primary and secondary peroxy radical populations, revealing a clear dependence on industrial preparation and irradiation conditions. We also assessed the effectiveness of different post-irradiation treatments in removing these radicals, identifying strategies with direct implications for limiting PFOA-precursor formation at the industrial scale. Complementary spectral simulations and pulsed EPR experiments (ESEEM, ENDOR) provided new insight into the nature of these radicals, resolving a previously unreported hyperfine coupling to fluorine nuclei and offering a first direct probe of their local chemical environment.

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Poster Abstract

Toward a Quantitative Assessment of Photoreactions by NMR

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Photo-induced chemistry currently experiences a vivid renaissance. By virtue of additive manufacturing and readily available LED light sources, a plethora of reactor designs has been realized. This variety highlights the importance of accurately describing the involved reaction conditions. Here, light intensity, penetration depth and kinetic aspects have to be considered. Unfortunately, many reported photoreactions suffer from non-sufficient data sets to enable a reasonable reproducibility.[1] NMR spectroscopy under light-irradiation can offer direct access to the relevant information on a structural level. A precise quantification however requires highly reproducible irradiation conditions not achieved in commonly used setups[2] (Figure 1).

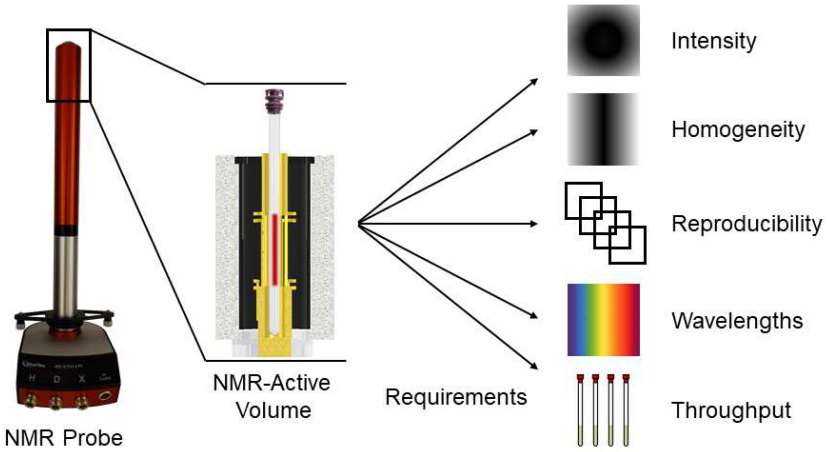

Figure 1. Photo-optical requirements within the NMR-active volume in light-irradiated NMR experiments.

We present a NMR probe with integrated light sources that provides strictly controllable photo-optical properties. It allows experiments under high-intensity light-irradiation to be performed routinely and at high throughput. By combining simulations and experimental methods, the light distribution within individual samples can be precisely described.[3] Utilizing this information, we will discuss how to quantify reaction parameters in the course of photophysical experiments. In doing so, we aim to provide basic guidelines on how to accurately plan and quantify photo-induced experiments.

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Poster Abstract

Optical Spin Polarization via Spin-Selective Charge Recombination in Luminescent Non-covalent TTM Diradicals

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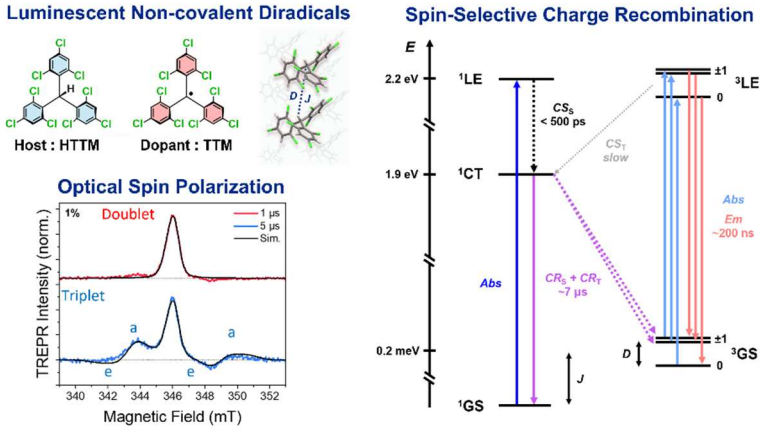
Molecular spin materials are promising platforms for quantum information science because their spin and optical properties can be tailored through molecular design. Tris(2,4,6-trichlorophenyl)methyl (TTM) radicals are attractive building blocks because they are stable, luminescent organic radicals with visible absorption and red photoluminescence[1]. Spin-selective optical polarization has also been demonstrated in covalently linked TTM diradicals[2].

Here, we generated luminescent non-covalent TTM diradicals by doping TTM radicals into crystals of HTTM, their diamagnetic hydrogenated analogue. Powder X-ray diffraction shows that 0.1–5 mol% TTM doping preserves the HTTM crystal packing, indicating isostructural replacement of HTTM molecules by TTM. Photoluminescence and transient absorption spectroscopy reveal that adjacent TTM radical pairs form a symmetry-broken charge-transfer state responsible that produces red-shifted, long-lived emission. Pulsed and time-resolved electron paramagnetic resonance (EPR) measurements confirm the formation of triplet diradicals and show that optical excitation polarizes their triplet ground-state sublevels through spin-selective charge recombination.

These results establish crystal doping as a simple strategy for generating noncovalent triplet diradicals and optically polarizing their spin states.



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[2] S. M. Kopp *et al.,* **J. Am. Chem. Soc.** 2024, 146, 27935–27945.

Poster Abstract

Theoretical Insights into Non-Equilibrium Spin Polarization in Triplet States through Lindblad dynamics

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Recent measurements on hyperpolarized triplet states of Jahn-Teller active porphyrins, where a long-lived net polarization was generated [1] and polarization transfer to a close-by radical was observed [2], highlighted once again how careful modeling of the system dynamics is required for interpreting Transient Electron Paramagnetic Resonance (TrEPR) spectra. In particular, as the initially photogenerated multiplet polarization on the triplet deviates strongly from equilibrium, the spin dynamics has to be described by a quantum master equation accounting for decoherence and dissipation eventually driving the systems to thermal equilibrium [3]. In the framework of open quantum system dynamics, the Lindblad Quantum Master Equation (LQME) allows to model virtually all the effects of the environment into the spin-dynamics. Thus, I will discuss a spectra simulation protocol based on the solution of LQME for spin dynamics and linear response theory [4]. This framework allows us to analyze how the relaxation processes shape the TrEPR spectra evolution. First, we recover the inversion of multiplet polarization caused by the interplay between spin-lattice relaxation and anisotropic phosporescent decay to the ground state. We then analyze how the lineshape is affected by dynamic Jahn-Teller effects, described as incoherent hopping between quasi-degenerate conformations [5]. Finally, we present some interesting transient effects in the spectral evolution.

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Poster Abstract

Ultrafast light control of magnetization dynamics in altermagnets

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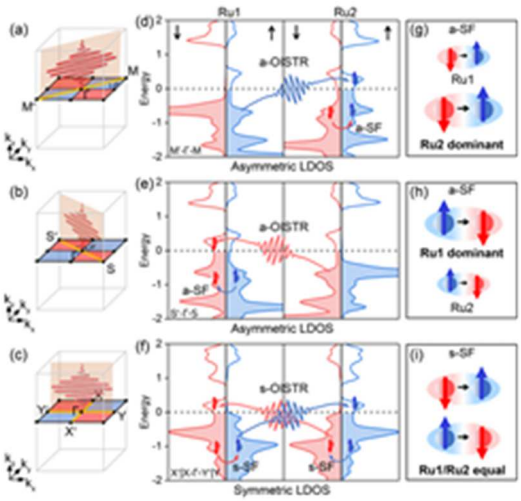
Altermagnets (AMs), featuring compensated magnetic order and momentum-dependent spin splitting, offer a promising platform for ultrafast optical control of spin without equilibrium net magnetization. Using real-time time-dependent density functional theory, we reveal that linearly polarized laser pulses can break sublattice symmetry and generate transient net magnetization in d-wave AMs RuO2 on femtosecond timescales. We observed that polarization-selective excitation drives pronounced asymmetric demagnetization between otherwise equivalent sublattices, producing a controllable ferrimagnetic state. This effect originates from asymmetric optical intersite spin transfer (OISTR), further enhanced by spin-flip processes, both governed by the nodal spin band topology [1]. Extending to g-wave AMs CrSb, we show that the magnetization dynamics strongly depend on the laser incidence direction, where oblique illumination induces sublattice asymmetry and net moments through anisotropic optical transitions [2]. Our results identify AMs as a versatile platform for ultrafast, all-optical spin manipulation.



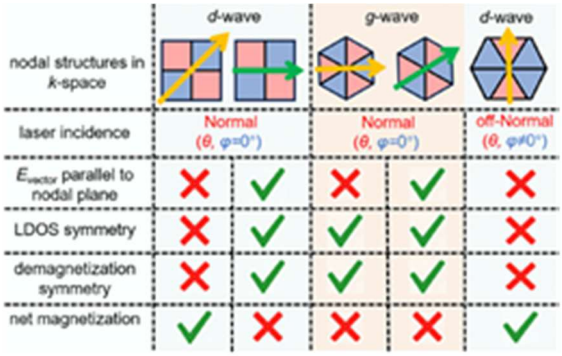


Figure 1. Plorization-dependent symmetric and asymmetric OISTR and spin flip (SF) mechanism in RuO2.
Figure 2. Summary of laser-driven asymmetric/symmetric demagnetization in d/g-wave AMs.

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Author Index

Author Index

E

F

G

H

I

J

K

L

M

N

O

P

Q

R

S

T

U

V

W

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