BRNO EFEPR CONFERENCE 2026

BRNO yEFEPR CONFERENCE 2026

13th European Federation of Electron Paramagnetic Resonance (EFEPR)

Book of Abstracts

29th Aug – 4th Sep 2026
Brno, Czech Republic

CEITEC | BRNO UNIVERSITY OF TECHNOLOGY | Groupement AMPERE

13th European Federation of Electron Paramagnetic Resonance (EFEPR) Conference, Brno, Czech Republic

Kolektiv autorů, sborník abstrakt

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Hlinky 48, 603 00 Brno
2026

yEFEPR 2026

	SATURDAY 29.08.2026		SUNDAY 30.08.2026	
08:00	Registration to yEFEPR			
08:15				
08:30				
08:45				
09:00	Opening of yEFEPR		Career Hour (Alice Bowen & James Eills)	S1 Chair: Orit Nir-Arad
09:15	Alice Bowen	S1 Chair: Sergei Kuzin		
09:30				
09:45				
10:00	Maria Chiara Pagliero		Coffee Break	
10:15	Shibnath Mandal (online)		Alysia Mandato	S2 Chair: James Eills
10:30	Shoaib Nazir (online)		Ivan Petkov	
10:45	Coffee Break		Olga Vojtíšková	
11:00			Tutorial 3 (Songi Han)	
11:15	James Eills	S2 Chair: Alex van der Ham		
11:30			Coffee Break	
11:45			DISCUSSION 1 "AI"	S3 Chair: Orit Nir-Arad & Alex van der Ham
12:00	Ayala Hecht			
12:15	Maya Rämisch			
12:30	Sudipta Khamrui			
12:45	Lubomir Loci		DISCUSSION 2 "Publishing"	S4 Chair: Sergei Kuzin
13:00	Lunch Break			
13:15				
13:30				
13:45			Closing yEFEPR	
14:00	Natalia Radzikowska	S3 Chair: Alice Bowen	Lunch Break	
14:15	Khuram Shehzad Khan			
14:30	Aistė Peštenytė			
14:45	Ikram Zdeg			
15:00	Aisika Chakraborty			
15:15	Saverio Canu		Meeting in front of the hotel	
15:30	Coffee Break		Tram leaves from "Výstaviště main entrance"	
15:45				
16:00	Muhammad Tahsin	S4 Chair: Lucie Kotásková & Jan Dubský	CEITEC Tours: – EPR laboratory – CEITEC Nano or Free Time	
16:15	Daina Arenas			
16:30	Tutorial 1 (Tomasz Czechowski)			
16:45				
17:00	Tutorial 2 (Petr Kostelník)			
17:15				
17:30	Mixer & Poster Session			
17:45				
18:00			Registration to main EFEPR conference	
18:15				
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EFEPR 2026

	MONDAY 31.08.2026		TUESDAY 01.09.2026	
08:00				
08:15				
08:30				
08:45				
09:00	Petr Neugebauer – Opening		Alexander Schnegg introducing Klaus Möbius	
09:15	Gunnar Jeschke	S1 Chair: Pierre Dorlet	Sabine Van Doorslaer	Klaus Möbius session S1 Chair: Alexander Schnegg
09:30				
09:45				
10:00	Bruno Guigliarelli		Orit Nir-Arad	
10:15			Alexey Bogdanov	
10:30	Paola Barbara		Roberto Zambon	
10:45	Mikhail Agrachev		Hugo Karas	
11:00	Coffee Break		Coffee Break	
11:15				
11:30	Stephen Hill	S2 Chair: Maria Fittipaldi	Alessandro Lunghi	S2 Chair: Sabine Van Doorslaer
11:45				
12:00	Songi Han		Ilia Kaminker	
12:15			Aharon Blank	
12:30	E. Kryukov (Cryogenic)		Dijana Žilić	
12:45	Lucca Sielaff		Alberto Cini	
13:00	Maxim Yulikov		Susanna Ciuti	
13:15	Lunch Break		Lunch Break	
13:30				
13:45				
14:00				
14:15				
14:30	Maxie Roessler	S3 Chair: Daniel Klose	Robert Bittl	S3 Chair: Mantas Šiménas
14:45				
15:00				
15:15	Susanne Mossin		Laura Galazzo	
15:30				
15:45	Jan Dubský		Lorenzo Sorace	
16:00	Lisa Ebo		Paolo Cleto Bruzzese	
16:15	Coffee Break		Coffee Break	
16:30				
16:45	Martina Huber	S4 Chair: Dana Dvoranová	M. Maylaender (Bruker)	S4 Chair: Petr Neugebauer
17:00				
17:15	Annemarie Kehl		Bela Bode	
17:30	Takuma Sato		General assembly	
17:45	Martin Dressel			
18:00				
18:15				
18:30	Poster Session 1 Odd numbers		Poster Session 2 Even numbers	
18:45				
19:00				
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21:00	Social Program		Social Program	
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EFEPR 2026

	WEDNESDAY 02.09.2026		THURSDAY 03.09.2026		FRIDAY 04.09.2026
08:00					
08:15					
08:30					
08:45					
09:00					
09:15	Martyna Elas	S1 Chair: Piotr Pietrzyk	Ilya Kuprov	S1 Chair: Inés García-Rubio	Sightseeing: − On Semi Co. − Conference Trip "Napoleon"
09:30					
09:45					
10:00	Periannan Kuppusamy		Fernando Luis		
10:15					
10:30	T. Czechowski (Novilet)		J. Sun (CIQTEK)		
10:45	Alberto Privitera		Maria Chrysina		
11:00	Coffee Break		Coffee Break		
11:15					
11:30	Athanassios Boudalis	S2 Chair: Oleksii Laguta	Emre Erdem	S2 Chair: Vinicius T. Santana	
11:45					
12:00	Jean-Gabriel Hartmann		Roberto Rizzato		
12:15	Valentin Novikov		Mathias Schubert		
12:30	Yasmin Ben-Ishay		Michal Zalibera		
12:45	Alexey Popov		Tomasz Kubiak		
13:00	Thierry Dubroca		Closing EFEPR		
13:15	Lunch Break		Lunch Break		
13:30					
13:45					
14:00			Meeting in front of the hotel		
14:15			Tram leaves from "Výstaviště main entrance"	Bus departs from the street outside the hotel	
14:30	City Tour / Free Time		CEITEC Tours: − EPR laboratory − CEITEC Nano then bus to: − NMR center − MRI facility	Fisher Scientific CZ Tour	
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19:00	Conference Dinner				
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Welcome to EFEPR 2026: From the roots of magnetic resonance in Brno to the future of EPR

Dear EPR Friends and Colleagues,

It is my great pleasure to welcome you to the **13th European Federation of Electron Paramagnetic Resonance Conference (EFEPR 2026)**, taking place in **Brno, Czech Republic, from 29 August to 4 September 2026**.

We look forward to welcoming colleagues from across Europe and beyond for a week of exciting science, stimulating discussions, new collaborations, and the opportunity to discover Brno. EFEPR 2026 is particularly special for us. **2026 marks 100 years since the birth of Professor Josef Dadok (1926–2024)** and, at the same time, **15 years of CEITEC – Central European Institute of Technology**. These two anniversaries provide a wonderful opportunity to celebrate Brno's remarkable history in magnetic resonance and its continuing contribution to the field.

From Josef Dadok to Rapid Scan EPR: The story of magnetic resonance in Brno is inseparably connected with Josef Dadok. After graduating from Brno University of Technology in the early 1950s, Dadok founded the Nuclear Magnetic Resonance Department at the Institute of Scientific Instruments of the Czechoslovak Academy of Sciences in 1960. At a time when access to advanced Western instrumentation was severely restricted, Dadok and his colleagues developed their own NMR technology [1–3]. The Institute's proximity to TESLA Brno enabled an exceptional collaboration between science and industry. In 1965, TESLA began serial production of Dadok's 60 MHz BS477 NMR spectrometer, making Czechoslovakia only the third country, after the United States and Japan, to achieve serial production of NMR spectrometers. Approximately 500 instruments were produced during the following 25 years [1,2]. Dadok later continued his scientific career in the United States, where he made further important contributions to magnetic resonance. Together with R. F. Sprecher, he published his influential work on Correlation NMR Spectroscopy in 1974 [4]. Their work introduced new approaches to acquiring and correlating magnetic resonance information and became an important contribution to the development of advanced NMR methodology. This scientific heritage provides a fascinating connection to the development of **Rapid Scan EPR**.

From Denver to Brno: Several decades later, Gareth R. Eaton, Sandra S. Eaton, and their colleagues at the University of Denver pioneered modern Rapid Scan EPR. Their work demonstrated that rapidly sweeping the magnetic field could provide EPR spectra on timescales far shorter than conventional continuous-wave measurements. Their developments in rapid-field scanning, resonators, detection, and signal processing established Rapid Scan EPR as a powerful experimental technique [5,6]. The Eaton group's work subsequently opened new possibilities for studying spin relaxation, transient phenomena, and EPR imaging [7]. The development of Rapid Scan EPR in Denver provided an important foundation for the subsequent development of frequency Rapid Scan EPR at high magnetic fields and frequencies by me and colleagues. In 2018, Laguta, Tuček, van Slageren, and I demonstrated rapid-scan EPR at 200 GHz, using extremely rapid frequency sweeps to access spin dynamics on the nanosecond timescale [8]. This work subsequently developed into the THz-FRaScan-ESR programme at Brno University of Technology and CEITEC, enabling rapid frequency-sweep EPR over a broad range of high frequencies and magnetic fields. For us, the connection to Dadok is particularly meaningful. His work on correlation NMR did not directly lead to Rapid Scan EPR, but it represents an important conceptual inspiration: the idea that new information can be

obtained by acquiring and correlating magnetic resonance signals in ways that go beyond conventional spectral acquisition [4].

15 Years of CEITEC: This story continues at CEITEC, which celebrates its 15th anniversary in 2026. Since its establishment, CEITEC has become an internationally recognized centre for interdisciplinary research. The Josef Dadok National NMR Centre at CEITEC, established in 2013, provides a particularly strong link between Brno's pioneering magnetic resonance history and today's research [3]. Our Magneto-Optical and THz Spectroscopy group is proud to contribute to this tradition through the development of high-frequency and frequency Rapid Scan EPR and related magnetic resonance technologies. EFEPR 2026 therefore brings together **100 years of Dadok, 15 years of CEITEC, and the continuing evolution of EPR**.

But above all, this conference is about people. We hope EFEPR 2026 will provide a place where established researchers can share their experience, young scientists can present new ideas, and collaborations can begin.

We warmly invite you to join us in Brno, to enjoy the science, the discussions, and the city—and to become part of this continuing story of magnetic resonance.

We look forward to welcoming you to EFEPR 2026!

Warm regards,

Petr Neugebauer
Chair of EFEPR 2026
CEITEC – Central European Institute of Technology
Brno University of Technology
Czech Republic

Prof. Josef Dadok at ENC 2006

References:

[1] B. Král and A. Blatná, *Slaboproudý obzor*, **72**, 4 (2016).

[2] V. Zeman, *Vzpomínky na NMR v Brněnské Tesle*. Stan's Library.

[3] J. Dubský et al., "ESR in the Czech Republic, its Historical Overview, Current Status, and Future," *Applied Magnetic Resonance* **55**, 1047–1064 (2024).

[4] J. Dadok and R. F. Sprecher, "Correlation NMR Spectroscopy," *Journal of Magnetic Resonance* **13**, 243 (1974).

[5] J. P. Joshi et al., "Rapid-Scan EPR with Triangular Scans and Fourier Deconvolution to Recover the Slow-Scan Spectrum," *Journal of Magnetic Resonance* **175**, 44–51 (2005).

[6] S. S. Eaton et al., "Rapid Scan Electron Paramagnetic Resonance," in *Multifrequency Electron Paramagnetic Resonance: Data and Techniques*, Wiley (2014).

[7] S. S. Eaton et al., "Rapid-Scan EPR Imaging," *Journal of Magnetic Resonance* **280**, 140–148 (2017).

[8] O. Laguta, M. Tuček, S. van Slageren, and P. Neugebauer, "Multi-frequency rapid-scan HFEPR," *Journal of Magnetic Resonance* (2018).

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Oleksii Laguta
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Plenary speakers

Robert Bittl
FU Berlin (DE)

Gunnar Jeschke
ETH Zürich (CH)

Maxie Roessler
QMU London (GB)

Sabine Van Doorslaer
Hasselt University (BE)

Martyna Elas
UJ Krakow (PL)

Ilya Kuprov
WIS Rehovot (IL)

Robert Bittl

Robert Bittl has studied physics at Technische Universität (TU) München (Germany) up to the doctorate (1988) working on the theory of stochastically modulated magnetic field dependent doublet pair spin dynamics. After a short stay at the University of Illinois at Urbana-Champaign (US) he worked as a postdoctoral researcher at Universität Stuttgart (Germany) on the electron paramagnetic resonance (EPR) spectroscopic detection of zero-quantum coherences after electron transfer in photosynthetic systems. This was initially theoretical work which led over to experiments at TU Berlin (Germany). There, he obtained the habilitation (1997) with work on time-resolved EPR to cofactor geometries in photosystems, in particular distances between cofactors.

Since 2001, he is professor for experimental physics at Freie Universität Berlin and applies a range of EPR spectroscopic methods to a variety of different problems in biological, chemical, materials, and medical physics. The methods include less-common variants e.g. electrically detected magnetic resonance and synchrotron-based frequency domain Fourier transform EPR. Examples for studied systems are blue-light photoreceptors, (catalytic) multi-nuclear metal centers, (in)organic photovoltaics materials, and Gadolinium-based magnetic resonance imaging contrast agents. More recently, he became interested in the chiral-induced spin selectivity effect, in particular its study by EPR methods on photo-induced donor-acceptor systems.

Gunnar Jeschke

Gunnar Jeschke studied chemistry at Technical University Dresden and graduated in 1992 with a thesis on analysis of sideband patterns in 31P solid-state NMR. Further stages were work on magnetic field effects on chemical reactions at RIKEN (Wako-shi, Japan), a doctoral thesis on new concepts in solid-state pulsed EPR (ETH Zürich, Switzerland 1996), solid-state NMR on inorganic materials (University of Bonn, Germany, 1997), and EPR studies on synthetic polymers and membrane proteins at MPI for Polymer Research (Mainz, Germany). Following appointment as full professor for physical chemistry at University of Konstanz (Germany) in 2006, he returned to ETH Zürich in 2008 as Full Professor for Electron Spin Resonance.

His research interests range from spin dynamics via EPR instrumentation to biophysics. Application work focuses on RNA-binding proteins and heterogeneous catalysis, while fundamental work focuses on electron spin decoherence due to the nuclear spin bath and ensemble structure determination of partially ordered proteins.

Maxie Roessler

Maxie Rößler is an Associate Professor in Chemistry and Director of the Centre of Pulse EPR spectroscopy (PEPR) at Imperial, London. She completed her DPhil with Prof. Fraser Armstrong FRS at the University of Oxford in 2012, took up a lectureship at Queen Mary University of London in 2013 and moved to Imperial in 2019, where she built up PEPR.

In her research she seeks to understand and exploit electron transfer reactions in chemical and biological systems. Her group combines EPR spectroscopy with electrochemistry, biochemistry and material science and has been developing film-electrochemical EPR spectroscopy as a new tool to gain mechanistic insights into complex metalloenzymes and electrocatalysts.

Recent awards include the Royal Society of Chemistry Joseph Black Prize (2024), the Imperial President's Medal for Excellence in Research (2023) and the European Bioinorganic Chemistry Medal (2022).

Sabine Van Doorslaer

Throughout her career, Sabine Van Doorslaer has been working at the interface between chemistry and (bio)physics. After obtaining a Master in Chemistry (1991), Master in Physics (1992) and PhD in Physics (1996) at Ghent University (BE), she worked as a postdoctoral researcher at ETH Zurich (CH) in the lab of Arthur Schweiger, till she was appointed as a professor at the University of Antwerp (BE) in 2002. From 2008-2024, she was also a guest professor at the University of Hasselt (BE).

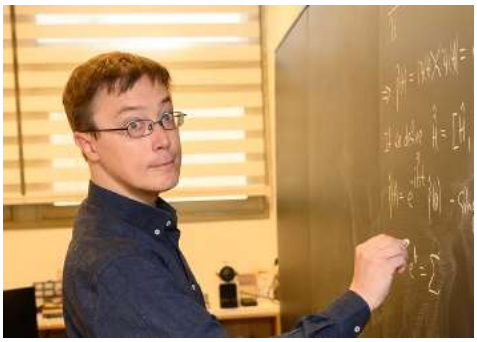
Her research is focussed on the development and application of EPR, with an emphasis on hyperfine spectroscopy. The EPR techniques are, where necessary, complemented with optical techniques and quantum-chemical methods. Her research group focusses on the characterization of a wide range of (bio)materials, including metalloproteins, homogeneous and heterogeneous catalysts and hybrid materials for applications in (bio)sensing, catalysis, membranes and organic (photo)voltaics. In 2018, she received the Bruker Prize granted by the ESR Spectroscopy Interest Group of the Royal Society of Chemistry.

Martyna Elas

My major interest is developing imaging methodology approach for studying tumor microenvironment. Electron Paramagnetic Resonance (EPR) oximetry, together with other tumor microenvironment parameters, such as oxidative stress, redox status, pH, allow broader approach to noninvasive studies of the tumor microenvironment. Tissue pO2 and hypoxia are our main focus. For example, we have shown that both hypoxia and vasculature play a role in tumor response to photodynamic therapy (Krzykawska et al., 2014), the role of vasculature changes in tumor tissue perfusion (Drzal et al., MRI 2022), or changes in the structure and function of the vasculature of tumors growing in the eye (Leszczynski et al., 2018). We also develop image analysis methods, such as co-registration of images acquired using different modalities (Gonet et al., 2019, Dziurman et al., 2025).

Today in our lab, we use EPR for pO2 determination, ultrasound for tissue structure, color Doppler ultrasound for blood flow, DCE-US and DCE-MRI for tissue perfusion, luminesce in vivo for metastasis development, and CT for tissue structure and metastasis. Recently, we have obtained optoacoustics imager, allowing the blood saturation measurements, as well as spatial distribution of collagen, melanin and other molecules. These noninvasive modalities are combined with molecular biology, confocal microscopy, and histology. Such a methodological approach allows us to study complex interactions within the tumor microenvironment and its role in tumor resistance to therapies. Our goal is to find out how the physical parameters of the tumor microenvironment, such as intratumoral pressure, perfusion, and pO2, interact with the biological factors and whether it is possible to modify these factors to achieve more effective antitumor therapies.

Ilya Kuprov



Professor Ilya Kuprov (Weizmann Institute of Science) is a specialist in theoretical modelling of spin dynamics and the principal author of Spinach software package that covers the whole of magnetic resonance spectroscopy and imaging. He has published over 120 papers and a book, mostly on theoretical and computational aspects of spin dynamics, and maintains a Magnetic Resonance education portal (https://spindynamics.org) with 100+ hours of lecture videos and 400+ pages of handouts. IK is also the physical sciences Editor at Science Advances, the open-access branch of the Science magazine.

Keynote speakers

Alessandro Lunghi
TC Dublin (IE)

Stephen Hill
NHMFL FSU Florida (US)

Athanassios Boudalis
CNRS Strasbourg (FR)

Fernando Luis
INMA Zaragoza (ES)

Susanne Mossin
DTU Lyngby (DK)

Laura Galazzo
ETH Zurich (CH)

Emre Erdem
SU IMC Istanbul (TR)

Periannan Kuppusamy
OSU Ohio (US)

Songi Han
Northwestern University (US)

Bruno Guigliarelli
Aix-Marseille Uni (FR)

Martina Huber
LU Leiden (NL)

yEFEPR speakers

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Forschungszentrum Jülich (DE)

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Petr Kostelník
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Tomasz Czechowski
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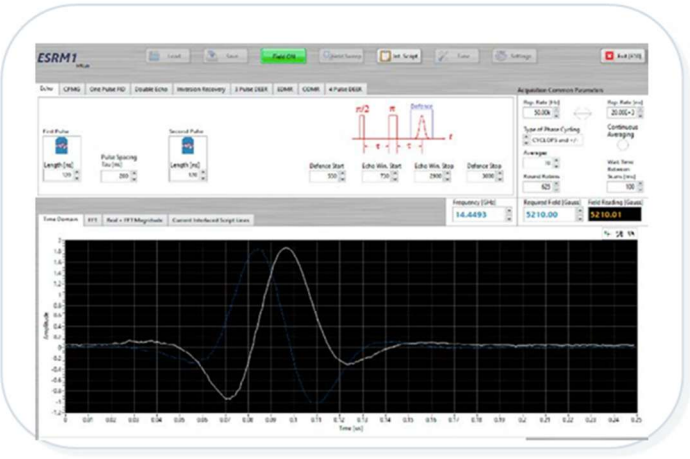

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BRNO

Welcome to Brno, the second-largest city in the Czech Republic and the vibrant capital of the South Moravian region. Strategically located at the crossroads of Prague, Vienna, and Bratislava, Brno blends deep historical roots with a forward-thinking, modern energy. It is remarkably defined by its youthful atmosphere, driven by a massive student population from the local universities that makes up nearly a fifth of the city's residents. This demographic keeps the historic, highly walkable center constantly alive with an independent spirit and an internationally renowned specialty coffee and gastronomy scene.

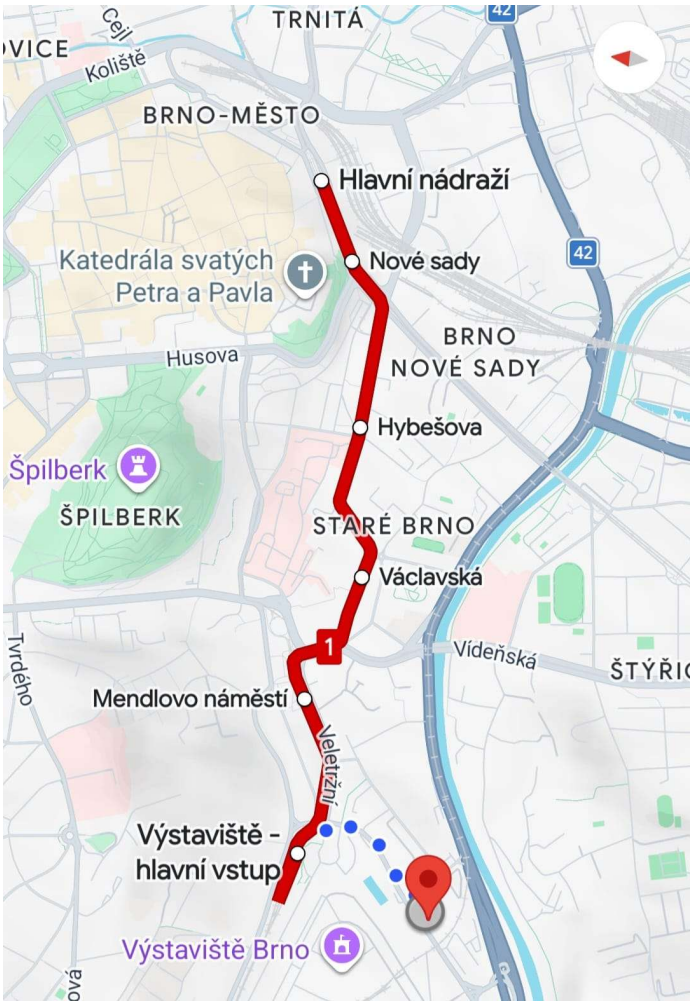
Beyond its rich cultural life, Brno is widely recognized as the Silicon Valley of Central Europe. It is a global powerhouse in the development and manufacturing of electron microscopes and serves as a major hub for international IT corporations, cybersecurity firms, and innovative tech startups. This technological prowess contrasts beautifully with the city's architectural heritage. Brno was a pioneering center for modernist architecture in the 1920s and 30s, most famously represented by the UNESCO-listed **Villa Tugendhat**, a masterpiece of functionalist design.

SCAN ME

How to get to the Orea Congress Hotel?

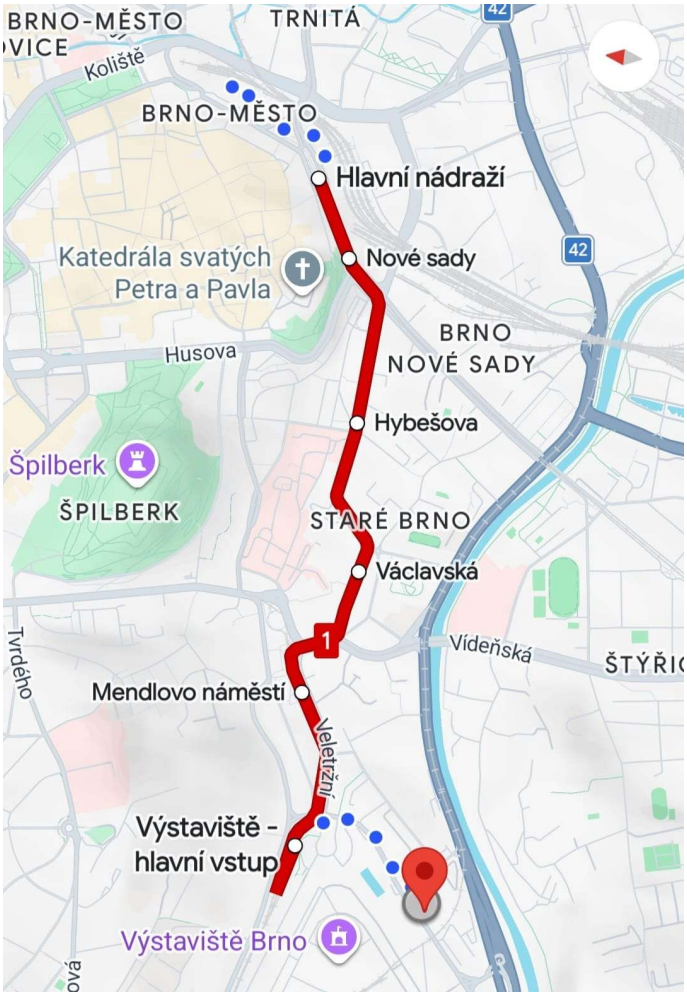
From Brno Main Train Station (Hlavní nádraží)

1. Walk out of the main station hall to the tram platforms directly in front of the building (to tram stop “Hlavní nádraží”).
2. Take **Tram line 1** (direction: Bystrc / Ečerova / Pisárky).
3. Ride **5 stops** to “**Výstaviště - hlavní vstup**” (~7 minutes).
4. Walk ~150 meters along **Křížkovského** street to the hotel.
   Total travel time: ~10 minutes



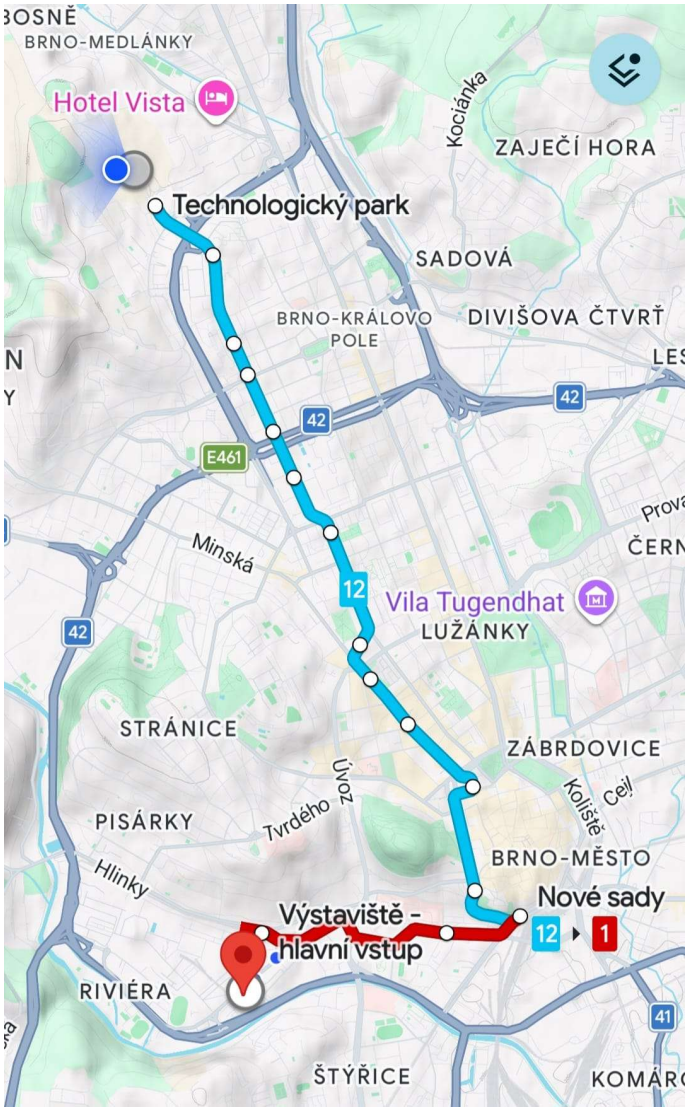
From Grand Bus Station (Autobusové nádraží u Grandu)

1. From the bus stop, walk ~200 meters (~2–3 minutes) south along **Benešova** street toward the main train station building.
2. At the **“Hlavní nádraží”** tram stop in front of the train station, take **Tram line 1** (direction: Bystrc / Ečerova / Pisárky).
3. Ride **5 stops** to **“Výstaviště - hlavní vstup”**.
4. Walk ~150 meters along **Křížkovského** street to the hotel.
   Total travel time: ~12 minutes



From CEITEC VUT

1. Walk ~100 m from CEITEC to the **“Technologický park”** tram stop (the terminal stop).
2. Take **Tram line 12** (direction: Komárov) and ride to **“Nové sady”** tram stop (~18 minutes).
3. At **Nové sady**, transfer to **Tram line 1** (direction: Bystrc / Ečerova / Pisárky).
4. Ride **4 stops** to **“Výstaviště - hlavní vstup”** (~7 minutes).
5. Walk ~150 meters along **Křížkovského** street to the hotel.
   Total travel time: ~30 minutes



Useful links:

Local public transport in Brno is operated by DPMB (https://www.dpmb.cz/en). Passengers can purchase tickets directly inside all trams, buses, and trolleybuses using a contactless payment card. For full details on the contactless system, please visit https://pipniajed.cz/en.html.

Practical information

Registration

Registration will be open from Saturday, 29 August 2026 throughout the conference period, at the Registration & Information Desk (cloak room, see map below) in the main foyer of the OREA Congress Hotel Brno. You will receive your registration pack and can collect your badge and conference materials there. Please see a member of the organising team if you need assistance.

Accommodation and meals

The conference venue is the OREA Congress Hotel Brno. All conference activities take place in the renovated congress centre, which is directly connected to the multifunctional foyer. Meals and coffee breaks are served partly in Hall A and partly in the foyer, exact times vary slightly from day to day depending on the programme; please see the conference book for details. Lunch is included in the cost of registration as indicated for your registration type. Breakfast and dinner arrangements depend on your booking day; participants who wish to join additional programs should speak to a member of the local organising team.

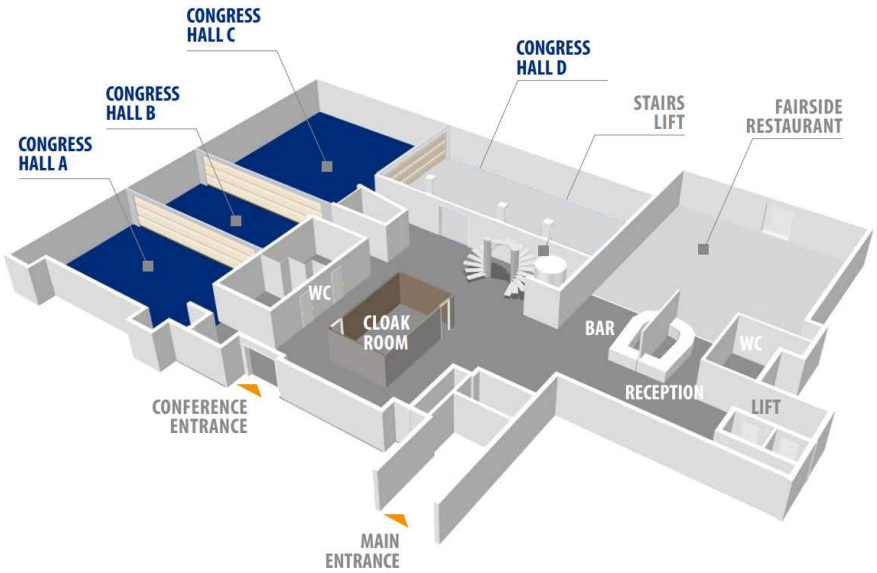
Lectures

Plenary and thematic sessions of the main EFEPR conference take place in Hall C, the largest central hall of the congress centre. Student sessions during the first two days are held in Hall B, adjacent to Hall A. Company and partner exhibitions are situated in Hall A, accessible directly from the foyer. Morning sessions start according to the programme published in this book.

Speaker information

Please allow time for discussion at the end of all lectures as indicated in the programme. A Windows PC with PowerPoint, Adobe Reader and a projector will be provided.

Speakers are kindly asked to upload their presentations onto the conference computer (and set up and test them) in the morning before the first session of the day of their presentation. It will also be possible to attach a speaker's own laptop to the projector; if this is strictly necessary, please provide any required display adapter. Members of the local organising team will be available to open the lecture hall and provide limited assistance. Please keep strictly to the time schedule for your talk.



General information

Poster presenter information

Poster presentations are displayed throughout the foyer of the congress centre, allowing easy access during breaks and transitions between sessions. Poster boards are A0 size. Please set up your poster after registration and keep it throughout the conference period (see the programme for odd/even numbering and session times). Posters should remain on display for the duration indicated in the programme and must be taken down by the end of the conference as announced by the organisers. Attachment materials will be provided at the registration desk. Poster numbers will be displayed on the boards. Coffee breaks and receptions will be held near the poster area.

Coffee breaks

Tea, coffee and refreshments are served during morning and afternoon breaks and during poster sessions, partly in Hall A and partly in the foyer. Please follow the times given in the programme.

Conference banquet and social events

Social events, including the conference banquet (if included in your registration), are listed in the programme with venues and start times. Please check your registration type for which events are included. Further details will be announced at the Registration & Information Desk.

Accompanying persons

There is no formal programme for accompanying persons, but the organising team can suggest places to visit in Brno and the surrounding area. For hotel facility queries please go to the hotel reception desk; for conference matters please speak to a member of the organising team.

Internet access

Wi-Fi is available throughout the OREA Congress Hotel. Login instructions are provided at check-in / in the registration pack. Please ask at the reception desk if you need assistance connecting.

Departure

Please vacate hotel rooms by the check-out time given by the hotel (typically 12:00) on your day of departure. Luggage storage can usually be arranged at reception until the end of the conference programme. The conference closes according to the final day schedule in this book.

Emergency information

Emergency services

In case of a medical, police, or fire emergency, **call 112**.

Medical cases

If you need urgent care outside office hours and cannot leave home, call **+420 545 538 538** — a doctor will visit you shortly. Otherwise go to Ponávka 6 (Mon–Fri 17:00–7:00; 24/7 on weekends and holidays). Emergency dental care is available there too.

Pharmacies

Most common medicines are available here, though not in every pharmacy. For evenings, nights, or weekends, use the 24-hour pharmacy at Koliště 47 in the city centre.

Police

The Czech Republic has two police forces: the National Police (Policie České republiky) and the Municipal Police (Městská policie). The National Police handle crime, traffic, and visas for foreigners. Municipal Police keep order locally and have more limited powers.

Post offices

Most post offices are only open on weekdays. On the opposite side of the Main Train Station remains open non-stop, 24 hours a day, seven days a week.

Emergency Medical Service	155	Fire Brigade	150
Municipal Police	156	National Police	158

Organization team (also WhatsApp)

Petr Neugebauer	+420734513280	Oleksii Laguta	+420777205116
Vinicius Santana	+420775898485	Lucie Kotásková	+420733226224
Eliška Dolejšová	+420775123512	Jan Dubský	+420775534010

BRNO
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2026

PLENARY LECTURES

EFEPR 2026 CONFERENCE
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Chasing Gadolinium Deposits in Biological Tissue

Robert Bittl,[1] Nicole Höfer,[1] Lina Anderhalten,[2] Daria Dymnikova,[1] Christian Teutloff,[1] Carmen Infante Duarte[2]

[1] Fachbereich Physik and Center for Chiral Electronics, Freie Universität Berlin; [2] Experimental and Clinical Research Center, A Cooperation Between the Max Delbrück Center for Molecular Medicine in the Helmholtz Association and Charité–Universitätsmedizin Berlin

robert.bittl@fu-berlin.de

The high-spin Gd^{3+} ion is used in magnetic resonance imaging (MRI) in the most common Gadolinium-based contrast agents (GBCA). Since Gd is highly toxic it is bound in the GBCA to chelators forming stable complexes. After intravenous injection, the GBCA are rapidly eliminated from the blood stream by renal clearance. Nevertheless, Gd deposition has been observed in different human tissues. [1] The type and duration of retention differ between linear or macrocyclic chelator and the specific tissue. While Gd retention of linear GBCA in brain seems to be permanent but non-permanent for macrocyclic GBCA. Inflammatory conditions of the tissue, e.g. in the chronic neuroinflammatory disease multiple sclerosis (MS), have been reported to increase Gd retention. An important question is whether all of the deposited Gd remains in the GBCA or to which extent Gd is released.

We use experimental autoimmune encephalomyelitis (EAE), a common mouse model of MS, to study GBCA retention and possible Gd release by EPR. Thereby, we apply high-frequency (94 GHz) EPR on sub-mm brain biopsy samples. Deconvolution of the cwEPR spectra recorded on a specimen treated with the linear GBCA gadopentetate revealed two components with characteristics of both GBCA-bound Gd^{3+} and Gd^{3+} in aqueous solution in a 7:3 ratio, indicating that *in vivo* some Gd dissociates from this linear GBCA. To further explore the local molecular environment of the retained Gd, we employed electron-nuclear double resonance (ENDOR) measurements. Gd-specific pulse ENDOR on tissue samples is hampered by strong signal contributions from endogenous paramagnetic species, in particular Mn^{2+}. We developed ENDOR sequences with tailored flip angles for different spin states, e.g. $S_{Mn^{2+}} = 5/2, S_{Gd^{3+}} = 7/2$, based on,[2] to efficiently suppress the unwanted signal contributions. The ^{1}H ENDOR measurements exhibited spectral features consistent with a partial Gd^{3+} release in case of the linear GBCA gadopentetate (Magnevist) while non release was observable for macrocyclic GBCA gadobutrol (Gadovist).[3]

This work has been supported by Deutsche Forschungsgemeinschaft – CRC 1340.

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An Overview of DNP and Hyperpolarization

James Eills

1Institutefor Structural Biochemistry, Forschungszentrum Jülich, 52428 Jülich

j.eills@fz-juelich.de

In 1953 Albert Overhauser predicted that saturating the conducting electrons in a metal would increase the polarization of the nuclear spins by three orders of magnitude,[1] a claim that was verified by Carver and Slichter in metallic lithium later the same year.[2] Seventy years on from this early dynamic nuclear polarization (DNP) experiment, the field of hyperpolarization has grown to include spin-exchange optical pumping (SEOP), parahydrogen-induced polarization (PHIP), and chemically induced dynamic nuclear polarization (CIDNP). These methods all prepare nuclear spins in a transient non-equilibrium state and routinely deliver signal enhancements of three to five orders of magnitude. In this talk I will review the various hyperpolarization methods.

I will then provide a tutorial review of DNP, and three experimental variants in widespread use today: liquid-state Overhauser DNP, dissolution DNP, and magic-angle-spinning DNP. We will cover the underlying electron-to-nuclear transfer mechanisms including the Overhauser effect, solid effect, cross effect and thermal mixing, and experimental factors such as polarizing agents, microwave sources, temperatures and magnetic fields used in practice. Finally, I will describe application areas of DNP such as materials characterization and clinical metabolic imaging.

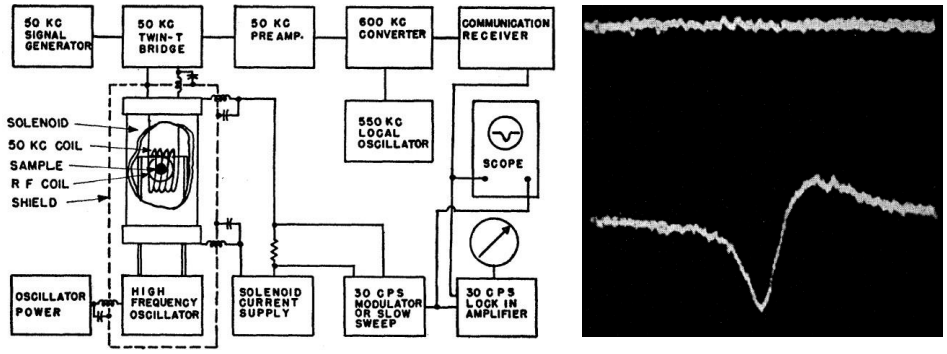

Fig.1: The apparatus used in the first DNP experiments on metallic ^{7}Li, and the HPNMR spectrum. [2,3]

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EFEPR 2026 CONFERENCE
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Quantitative EPR oxygen mapping in preclinical tumors – challenges and perspectives

Aleksandra Bienia[1,2], Aleksandra Murzyn[1,2], Gabriela Dziurman[1,2], Bartosz Płóciennik[1,2], Piotr Świerzewski[1,2], Małgorzata Szczygieł[1], Agnieszka Drzał[1], Martyna Krzykawska-Serda [1], Martyna Elas[1]

[1]Jagiellonian University, Faculty of Biochemistry, Biophysics and Biotechnology, Department of Biophysics and Cancer Biology, Kraków, Poland; [2]Doctoral School of Exact and Natural Sciences, Jagiellonian University, Krakow, Poland

martyna.elas@uj.edu.pl

Quantitative assessment of the tumor microenvironment (TME) requires high-resolution data on absolute oxygen partial pressure (pO_2) and redox status. EPR remains the gold standard for these measurements; however, the choice between Continuous Wave (CW) and Pulse EPR methodologies significantly impacts the spatial and temporal fidelity of the resulting data.
Three distinct EPR approaches applied to preclinical tumor models of uveal melanoma, breast cancer and glioma were used. First, we detail the use of CW EPR with solid-state probes (LiNc microspheres and OxyChip), demonstrating its optimality for repeated, longitudinal point-measurements in high pO_2 environments. Second, we explore Pulse EPR Oxygen Imaging (EPROI) utilizing the IRESE (Inversion Recovery Electron Spin Echo) pulse sequence with soluble trityl radicals (OX071). This approach yields 4D oximetry maps with very good spatial and oxygen resolution, allowing for the characterization of oxygen topologies. Third, we address redox characterization through the bioreduction kinetics of nitroxide probes (3-carboxy-proxyl), which provide a secondary layer of TME information when analyzed alongside oximetry.
Finally, we discuss the integration of these EPR techniques with anatomical and functional ultrasound (Doppler) imaging to register pO_2 maps with tumor anatomy and active vasculature. Our results suggest that while CW methods are ideal for monitoring therapy-induced changes over time, pulse EPR provides the essential 3D context required to understand TME heterogeneity and dynamic responses to novel therapies like oxygen microbubbles.

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Electron Spin Decoherence in the Low-Temperature Regime

Gunnar Jeschke[1]

[1] ETH Zürich, Department of Chemistry and Applied Biosciences, 8093 Zürich, Switzerland

gjeschke@ethz.ch

All EPR measurements depend on lifetimes of coherences and of non-equilibrium polarization on electron-spin transitions. These lifetimes in turn depend on fluctuations of the system's spin Hamiltonian parameters and of its couplings to the environment. However, at sufficiently low temperatures coherence decay (or decoherence) is usually dominated by static couplings of the electron spins in the system of interest to spins in the environment. This low-temperature regime is of particular interest, as most pulsed EPR and quantum sensing experiments are carried out in there.

Three major contributions to decoherence arise in this regime that spread the electron-spin coherence to nuclear-spin clusters, to quantum-rotor tunnel transitions, and to other electron spins. For Hahn-echo decay, the first contribution can be computed extremely fast with only small error as a product of analytical expressions for nuclear spin pairs coupled to the electron spin [1]. The second contribution arises mostly from methyl protons. Its prediction requires knowledge of the rotation barrier of the methyl groups, with density functional theory computations giving reasonable, but not perfect results [2]. The third contributions is confusingly called instantaneous diffusion and is usually avoided by dilution of the electron spins. In systems where high local electron-spin concentrations cannot be avoided, it dominates.

All three contributions can be suppressed to some extent by refocusing schemes, which is called dynamical decoupling. Both repeated π pulses [3] and spin-lock [4,5] prolong coherence lifetime for decay induced by nuclear-spin clusters and quantum rotors. Dynamical decoupling for dense electron baths requires to intersperse π pulse refocusing with solid-echo refocusing.

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What exactly is spin?

Ilya Kuprov

Department of Chemical and Biological Physics, Weizmann Institute of Science

ilya.kuprov@weizmann.ac.il

This tutorial lecture will explore the fundamental question of how spin comes to exist.

First, we will look at how group theory may be used to turn reasonable assumptions about physical reality (causality, uniformity, continuity, *etc.*) into equations of motion and conservation laws. Then, after a brief review of special relativity and Lorentz transforms, we will use the same methods to show that angular momentum conservation laws are different in Euclidean space and in Minkowski space-time. The difference is called spin.

We will then derive Dirac's equation and demonstrate how electron Zeeman interaction, spin-orbit coupling, and other components of the Pauli Hamiltonian turn up. If we have time, we would also look at nuclear spin (which isn't actually spin in the same sense as for the electron), nuclear magnetic moment, and nuclear quadrupolar interaction.

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EPR at the Interface: From Operando Spectroelectrochemistry to Superconducting Microresonators

Maxie M. Roessler[1]

[1] Imperial College London, Department of Chemistry and Centre for Pulse EPR Spectroscopy (PEPR); 82 Wood Lane, London W12 9QQ, United Kingdom

m.roessler@imperial.ac.uk

EPR is uniquely suited to probing unpaired electrons and transient intermediates, yet many chemically important systems remain challenging because the spins of interest are located at interfaces, present in low numbers, or evolve under operating conditions. In this lecture I will discuss recent advances that extend the reach of EPR towards these regimes.

First, I will present the development of film-electrochemical EPR (FE-EPR) platforms[1] based on free-standing single-walled carbon nanotube buckypaper electrodes.[2] These highly conductive, low-loss electrodes overcome challenges associated with combining electrochemistry and EPR, enabling operando spectroelectrochemical measurements across a wide potential and pH range. The approach allows direct observation of surface-bound radical intermediates and reaction kinetics under catalytic turnover, providing new insight into electron-transfer processes at electrode interfaces.

In the second part, I will discuss the development of high-temperature superconducting microresonators for pulse EPR spectroscopy of volume-limited samples.[1] By improving sensitivity while reducing sample requirements, these micrometre chips enable measurements on ultrathin films containing only ~10^{11} paramagnetic centres. Applications ranging from model copper-containing materials to metalloproteins demonstrate how advanced pulse EPR methods can be brought to previously inaccessible systems.[4]

Together, these developments are transforming EPR from a predominantly bulk characterisation tool into a technique capable of interrogating spins at surfaces, interfaces, and in thin films. In doing so, they open new opportunities to investigate the molecular mechanisms of catalysis, energy conversion and biological function.

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Elucidating different stages in the design of bio-based hybrids using EPR

Sabine Van Doorslaer,[1] Andrea Guidetti,[1,2] S. Fardokht Rezayi,[1,2] Lore Van den Bergh[1,3], Charlotte Simms[1,3], Norbert Lihi,[4] Nóra V. May,[5] Rui An,[3] Vera Meynen,[3] H. Y. Vincent Ching,[1] and Damien M. Murphy[2]

[1] University of Antwerp, Department of Chemistry, TSM[2], 2610 Antwerp, Belgium; [2] School of Chemistry, Cardiff University, Park Place, Cardiff CF10 3AT, United Kingdom; [3] University of Antwerp, Department of Chemistry, LADCA, Antwerp, Belgium; [4] University of Debrecen, HUN-REN-UD Mechanisms of Complex Homogeneous and Heterogeneous Chemical Reactions Research Group, Department of Inorganic and Analytical Chemistry, H-4032 Debrecen, Hungary; [5] Centre for Structural Science, Research Centre for Natural Sciences, Hungarian Research Network (HUN-REN), H-1117 Budapest, Hungary

sabine.vandoorslaer@uantwerpen.be

Transition-metal containing proteins exhibit a rich chemistry with a high activity and selectivity that is of interest for many applications, such as biocatalysis, bioremediation, medicine and biosensing. Unfortunately, the direct use of these proteins is often limited because of their instability under the application conditions. To circumvent these problems different routes are considered. On the one hand, the biomolecules can be immobilized in or on synthetic (porous) matrices resulting in hybrids in which the confinement conditions allow for longer protein stability and can even help to tune protein activity. On the other hand, synthetic low-molecular-weight transition-metal complexes, so-called synzymes, can been designed to mimic the protein's function. Subsequent incorporation of these complexes in porous materials can in turn lead to novel materials with unsurpassed properties. Although these approaches are very promising in theory, the actual design of these materials turns out to face many hurdles. In this talk, I will use examples from our research to outline how a broad scala of EPR techniques can be used to understand different stages in the development of hybrid material and/or synzymes. This will include the use of hyperfine techniques to link structural flexibility to activity of synzymes [1], the application of high-field spin-probe EPR to understand surface properties of functionalized titania supports [2] and the use of dipolar spectroscopy and/or hyperfine spectroscopy to observe structural changes in heme proteins and small transition-metal complexes when incorporated in porous materials, such as titania and zeolites.

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KEYNOTE LECTURES

EFEPR 2026 CONFERENCE
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EPR Spectroscopy of Defects in Nanomaterials for Energy Storage

Emre Erdem[1]

[1] Faculty of Engineering and Natural Sciences, Sabanci University, 34956, Tuzla, Istanbul, Türkiye

emre.erdem@sabanciuniv.edu

Electron paramagnetic resonance (EPR) spectroscopy provides a direct and highly sensitive probe of paramagnetic defect states and their local electronic environments. In this presentation, I will discuss how multi-frequency EPR spectroscopy, complemented by photoluminescence (PL), can be used to identify and understand intrinsic and extrinsic defects in functional nanomaterials, with examples from semiconductor ZnO, ferroelectric and lead-free perovskites, and two-dimensional materials.

Selected examples will demonstrate how EPR reveals ion substitution, charge-compensation mechanisms, oxygen vacancies, and local structural distortions, as well as the effects of doping, nanoscale confinement, thermal treatment, and photoexcitation on defect states. Particular attention will be given to ZnO nanostructures, where EPR and PL allow surface and bulk defects to be distinguished and correlated with changes in the electronic and optical properties of the material.

The main part of the presentation will focus on how this defect-level understanding can be translated into improved energy-storage performance. ZnO nanostructures characterized by EPR and PL will be employed as electrode materials and integrated into supercapacitor devices, providing a direct link between defect populations and electrochemical behavior. We will show how nanoscale morphology and defect engineering can enhance charge storage, charge-transfer kinetics, capacitance, energy and power densities, and cycling stability. Examples from lead-free perovskites and two-dimensional materials will further illustrate how controlling the local defect environment can be used to optimize electrode functionality.

Overall, the presentation will demonstrate how EPR spectroscopy can bridge microscopic defect physics and macroscopic device performance (here supercapacitors), providing a powerful approach for the rational design of nanomaterials for next-generation energy-storage technologies.

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Probing disorder and phase separation in RNA-binding proteins by EPR spectroscopy

L. Galazzo[1], N. Kociolek[2], K. Packebusch[1], M. Yulikov[1], F.H.T. Allain[2], G. Jeschke[1]

[1] Institute of Molecular Physical Science, ETH Zürich, Zürich, Switzerland; [2] Institute for Biochemistry, ETH Zürich, Zürich, Switzerland

laura.galazzo@phys.chem.ethz.ch

Over the past decade, intrinsically disordered regions have emerged as central determinants of the assembly and function of RNA-binding proteins [1]. Many of these proteins undergo liquid-liquid phase separation (LLPS) in response to stress, and the reversibility of this process is intimately linked to pathological dysfunction [2]. Deciphering their mechanisms of action therefore requires detailed insight into their structural and dynamic properties. For proteins that lack a well-defined three-dimensional fold, EPR spectroscopy provides a powerful strategy to map conformational landscapes and derive structural information from distance restraints [3].
Here, we focus on the RNA-binding protein Serine/Arginine-Rich Splicing Factor 1 (SRSF1) [4], a member of the SR protein family of gene regulators. SRSF1 contains two RNA-recognition motifs (RRMs) connected by a flexible linker, and a C-terminal disordered serine/arginine-rich tail (RS domain). While the RRMs mediate specific protein-RNA interactions, the RS domain is involved in protein-protein interactions and non-specific protein-RNA contacts, and it drives phase separation. Phosphorylation of the RS domain is essential for correct protein localization and function. For this protein, a combination of EPR and NMR has been used to unravel structural details of SRSF1 in its apo state, bound to a short RNA and upon phosphorylation.
The challenges associated with performing EPR experiments on phase-separated samples will be also addressed. Under these conditions, high local concentrations and fast relaxation rates impose fundamental limitations on the quantity and reliability of structural information that can be extracted.
In addition, a novel strategy for the site-selective spin labelling of proteins containing structurally relevant cysteine residues will be introduced. This approach exploits intein-mediated protein trans-splicing (PTS) [5] and is demonstrated on the intrinsically disordered protein Fused in Sarcoma (FUS). Thanks to this method, the N-terminal domain of full-length FUS, which contains a zinc finger accessible to conventional spin labels, was selectively labelled, circumventing cysteine mutagenesis that would otherwise impair RNA binding.

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W-formate dehydrogenases: The best enzymes to crunch CO_2?

B. Guigliarelli,[1] F. Biaso,[1] M. Seif Eddine,[1] G. Gerbaud,[1] AR. Oliveira,[2] RR. Manuel,[2] G. Vilela-Alvez,[3] C. Mota,[3] MJ. Romão,[3] IC. Pereira[2]

[1]Aix Marseille Univ, CNRS, Bioénergétique et Ingénierie des Protéines, Marseille, France; [2]Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Oeiras, Portugal; [3]UCIBIO, Department of Chemistry, Universidade Nova de Lisboa, Caparica, Portugal

guigliar@imm.cnrs.fr

Molybdenum (Mo) and tungsten (W) enzymes are found in virtually all living organisms where they catalyze a wide diversity of redox reactions. In prokaryotes, most of these enzymes harbour a large Mo/W-*bis* pyranopterin guanosine dinucleotide cofactor in which the metal ion cycles between the +IV and +VI redox states during catalysis. However, in spite of numerous crystallographic and spectroscopic studies, the structure of active site intermediates and catalytic mechanisms are still largely debated. In the case of the +V redox state which is detectable by EPR, several species are often detected and their relationships with structural data, enzyme activity and catalytic intermediates remain unclear.

The formate dehydrogenase (FdhAB) isolated from the bacterium *Desulfovibrio vulgaris* Hildenborough is a W and SeCys dependent enzyme showing remarkable properties of CO_2 reduction and O_2 tolerance[1]. Depending on substrate or reductant used, several W(V) species could be observed and in parallel several X-ray crystallographic structures were obtained for the different redox or activity states of the enzyme. By using a combination of site directed mutagenesis, EPR analysis of enzyme preparations both in solution and in crystal state, relationships between these species and enzyme active forms could be established [2]. Moreover, by combining *g*-tensor and hyperfine coupling analysis (^{183}W), isotope labeling (^{77}Se) and DFT calculations, structural models of these species could be obtained. The results indicate clearly that the SeCys remains bound to the W ion throughout the catalytic cycle, clarifying a long debate [3].

More recently, the protonation state of the W-center was also investigated by HYSCORE spectroscopy and surprising differences were found with homologous Mo-Fdh. This reveals notable differences between the catalytic mechanisms of the two kinds of enzyme which could explain their striking difference of reversibility in the catalyzed reaction.

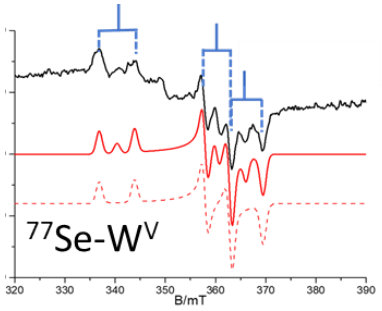

Figure 1: EPR spectrum of ^{77}Se-labelled W-Fdh (simulations in red).

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Active Role of Water in Protein Assembly and Function

Songi Han

Department of Chemistry, Northwestern University, Evanston, Illinois, USA; Department of Chemistry and Biochemistry, University of California, SantaBarbara, California, USA; Department of Chemical Engineering, University of California, Santa Barbara, California, USA

songi.han@northwestern.edu

Water is central to how biological molecules interact, assemble, and perform chemical and biological work, yet it remains exceptionally difficult to characterize. It behaves as both a liquid and a structured material, adopting multiple distinct configurations around dissolved solutes. A combination of ^{1}H and ^{17}O nuclear magnetic resonance and electron-nuclear double resonance spectroscopy can resolve the dynamical, structural, and thermodynamic properties of water as they vary with the surface chemistry and topology of small molecules and biological macromolecules. I will outline the measurement principles and why they are not yet routinely applied and discuss the conditions under which the shaping of water occurs and why it matters for biomolecular function. Control experiments with DMSO, glycerol, and phosphate reveal that even these "simple" mixtures carry rich and unexpected structural signatures of their own. I will showcase the importance of teasing out the property of water associated with proteins to track molecular assembly, shape directed protein assembly, protein activation to protein-based signal transduction.

One example I will highlight is our discovery of water-mediated pinning hotspot that drive templated aggregation of tau. Tau proteins must align and stack precisely with existing fibril ends to propagate pathology, yet the molecular signature that initiates and ensures this in-register alignment has been unclear. We show that recruitment begins at a single, structurally well-defined contact site on the fibril surface that is enriched in release-prone hydration water. These findings reveal that water-release-prone hotspots, rather than the well-known amyloid-core regions alone, govern the initial steps in templating seeding and can hence be blocked, opening a new path for identifying therapeutic targets that could slow the progression of tau-related diseases. These studies required a combination of EPR, Overhauser DNP and NMR tools, with each method offering unique insight.

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Wideband Multiphoton ESR in Multilevel Gd^{3+} Spin Qudits

Stephen Hill,[1,2] Sabastian I. Atwood,[1] Manoj Subramanya,[1] Xiao Chen,[3] Andrew Cupo,[3] Tomas Orlando,[1] Hai-Ping Cheng[3]

[1] National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, United States; [2] Department of Physics, Florida State University, Tallahassee, FL 32306, United States; Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306, United States; [3] Department of Physics, Northeastern University, Boston, MA 02115, United States

shill@magnet.fsu.edu

Electronic systems with large spin quantum numbers have been proposed for efficient information storage and retrieval using a Grover-like quantum search algorithm [1]. In this proposal, an *N*-state electron spin system functions as an *N*-bit register in which information is stored in the quantum phase of each state and read out with standard pulsed electron spin resonance (ESR) spectroscopy. High-spin systems offer multiple quantum spin levels and strong coupling with electromagnetic radiation. However, they are also subject to the well-known selection rule that formally restricts changes in spin projection to a single quantum, so that creating a superposition of nonadjacent spin states is forbidden to first order. Multiphoton absorption, a nonlinear process, presents a solution, as has been demonstrated in ESR spectroscopy on the highly symmetric cubic system Mn^{2+}:MgO [2]. Using pulsed high-power ESR spectrometers at the National High Magnetic Field Laboratory [3], we demonstrate coherent two- and three-photon absorption in the less symmetric tetragonal system Gd^{3+}:YVO_4, the crystal symmetry of which allows tuning of the virtual state that controls the transition rate. Furthermore, we demonstrate coherent control of two-photon transitions using two-tone microwave excitation, in which the microwave frequency rather than the crystal orientation controls the virtual state. These results show that the study of quantum memory schemes is not limited to high symmetry systems, paving the way for demonstration of a quantum search algorithm in a high-spin Gd^{3+} system.

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Electric-field EPR, magnetoelectric phenomena and symmetry breaking in molecular materials

Athanassios K. Boudalis,[1] Jason S. R. McCoombs,[1] Jorge I. Hilari,[1] Jérôme Robert,[2] Filippo Troiani[3]

[1]Institut de Chimie UMR7177 (Université de Strasbourg-CNRS), 4 rue Blaise Pascal, Strasbourg, France; [2]Institut de Physique et Chimie des Matériaux de Strasbourg UMR7504 (Université de Strasbourg, CNRS), 67000 Strasbourg, France; [3]Centro S3, CNR-Istituto di Nanoscienze, I-41125 Modena, Italy

bountalis@unistra.fr

Magnetoelectricity refers to changes in the electric polarization of matter due to magnetic fields, or, *vice versa*, to changes in its magnetization due to electric fields.

Very recently, it has re-emerged in the domain of Magnetic Resonance through the perspective of constructing electrically controllable molecular spin qubits, either based on single spins[1] or on spin-chiral triangles.[2] In the latter case, this interest led for the first time to the electrical addressing of multispin exchange-coupled systems,[3] as previous studies mainly revolved around dilute paramagnetic impurities.[4] This has introduced new terms to ME models, such as Heisenberg and Dzyaloshisnkii-Moriya exchange, also relevant in multiferroics research, necessitating the revision of prior symmetry-related arguments.

Indeed, we have found that the ferric triangle $[Fe_3O(O_2CPh)_6(py)_3]ClO_4 \cdot py$ (**Fe$_3$**), which crystallizes in the centrosymmetric space group $P6_3/m$, shows significant changes of its CW EPR signal under static E-fields,[3] as corroborated through non-resonant magnetometry.[5] Subsequent dielectric measurements conducted under modulated magnetic fields revealed an electrically-detectable first-harmonic ME effect, in principle not allowed by symmetry.[6]

Here, we will present an analysis of these results in view of recent Electric-Field Modulated EPR (EFM-EPR) studies, outlining possible mechanisms that could break the fine balance of symmetry elements allowing the observation of such signals.

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EPR approaches to intrinsically disordered proteins and metal-ion centres related to neurodegenerative disease.

Martina Huber

Department of Physics, Huygens-Kamerlingh Onnes Laboratory, Leiden University, Niels Bohrweg 2, 2333CA Leiden, The Netherlands

huber@physics.leidenuniv.nl

There are many examples, where EPR can give insight into biological questions that are inaccessible by other techniques. Here, protein-protein interactions, the elucidation of the electronic structure of active centres in proteins, and the determination of protein dynamics and -structure are important examples.

The self-aggregation of amyloid proteins is discussed as a possible cause of neurodegenerative disease. While the end product of this aggregation are the β-sheet amyloid fibrils that form the plaques in the brain, aggregation intermediates, the so-called oligomers, may be the toxic species that cause nerve cells to decay. Amyloid proteins are intrinsically disordered proteins (IDP's), so they lack a stable fold and are highly flexible, making them difficult to study. We will discuss examples of how we follow the aggregation (Fig. 1) and interactions of these proteins by EPR.

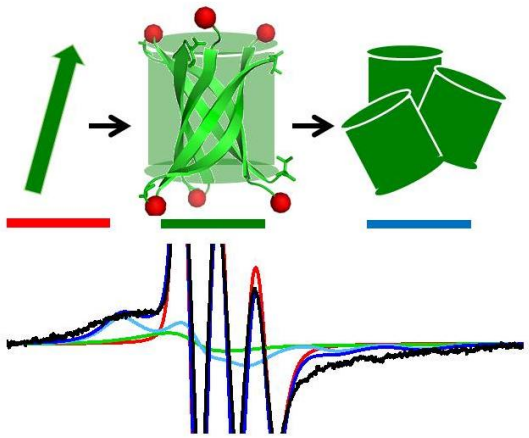

Fig 1. Amyloid aggregation by cw-EPR. Model peptide with fixed TOAC spin label for oligomer intermediates [1]

Also discussed is the involvement of metal-ions in the disease, where iron imbalance in the brain may be a causative factor. We showed that different metal-forms can be detected in brain material [2-4] and started on an in-depth investigation of ferritin, the main iron-storage protein in the organism [5].

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Advancing EPR Technology for Quantitative Tissue Oximetry: From Molecular Probes to Clinical Devices

Periannan Kuppusamy

Geisel School of Medicine at Dartmouth College, 1 Medical Center Drive, Lebanon, New Hampshire, USA

periannan.kuppusamy@dartmouth.edu

Quantitative measurement of oxygen in living tissues is an important biomedical need and a demanding technological challenge for electron paramagnetic resonance (EPR). Advances in oxygen-sensitive probes, resonator design, magnetic-field generation, signal detection, and instrumentation have transformed EPR oximetry from a laboratory method into a versatile platform for in vivo oxygen measurement and imaging. This lecture will highlight enabling EPR technologies that improve sensitivity, measurement depth, portability, and clinical accessibility.

Stable oxygen-sensitive paramagnetic probes provide quantitative measurements of tissue partial pressure of oxygen (pO_2). Implantable sensors, including OxyChip, enable repeated measurements from the same tissue location. Advances in surface and dielectric resonators, implantable resonant structures, and minimally invasive detectors have further expanded the capabilities of in vivo EPR. Co-optimization of the spin probe, resonator, detection geometry, and magnetic-field environment has been critical to improving measurement performance.

Recent developments have focused on reducing the size and complexity of EPR systems. OxyTrack, a minimally invasive needle-based EPR oximetry platform, brings the resonator and oxygen-sensitive material directly to the tissue, enabling localized pO_2 measurements with substantially reduced RF power requirements. Emerging designs incorporate miniature permanent magnets with the sensing geometry, moving toward compact EPR devices in which the magnetic field, resonator, and oxygen sensor are integrated. Together with low-power RF electronics and compact instrumentation, these developments offer a pathway toward portable, point-of-care EPR systems.

A complementary direction is the integration of EPR oximetry with oxygen-enhanced MRI (OE-MRI). Quantitative EPR measurements can provide pO_2 reference information for calibrating MRI oxygen responses, enabling quantitative OE-MRI (qOE-MRI) and high-resolution maps of absolute tissue oxygenation. This approach combines the quantitative accuracy of EPR with the spatial coverage and anatomical resolution of MRI for multiscale oxygen imaging

Collectively, these advances illustrate a transition from adapting conventional spectrometers for in vivo measurements toward purpose-built biomedical EPR technologies. Continued innovation in probes, resonators, magnets, RF electronics, and multimodal integration should enable increasingly compact and clinically deployable systems for quantitative oxygen sensing, real-time tissue oxygen monitoring, and ultimately oxygen-guided diagnostics and therapy.

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Wiring up molecular spins with quantum superconducting circuits

Fernando Luis[1]

[1] Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, 50009, Zaragoza (Spain)

fluis@unizar.es

Scaling up quantum processors remains very challenging, even for today's most successful platforms, on account of the need of mitigating errors. Magnetic molecules provide competitive advantages, due to their exquisite reproducibility and the ability of tuning relevant properties and of scaling up quantum resources by chemical design [1]. Exploiting them calls for a solid-state platform able to initialize, control and read-out the spin states and of establishing remote communication channels [2]. I'll discuss recent experiments aimed at achieving this goal by circuit QED techniques, coupling molecular spins to chips hosting multiple *LC* superconducting resonators [3]. Results on molecular ensembles provide proof-of-concept implementations of basic quantum operations on both electronic and nuclear spins [4]. We also find that the circuit mediates effective interactions between remote spin ensembles located on separately addressable resonators [5]. Finally, I'll discuss strategies, based on optimizing the circuit or the molecular integration, for extending this approach to reach coherent coupling of mw cavity photons to individual molecular spins [4,6].

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An ab initio theory of spin decoherence in magnetic molecules

Alessandro Lunghi[1]

[1] School of Physics, CRANN Institute, Rinn Quantum, Trinity College, Dublin 2, Ireland

lunghia@tcd.ie

Magnetic molecules play an important role in several applications, going for magnetic resonance tags to potential elements of quantum information technology. At the heart of their working mechanism there is the possibility of creating and manipulating highly coherent superpositions of their spin states. As such, understanding the physics behind the quantum properties of molecules represent an important scientific goal with the potential of improving the coherence of such systems. In this contribution we will provide an account of how ab initio simulations have allowed, over the last 10 years or so, to establish a microscopic understanding of the processes underpinning the physical limits of spin coherence in molecules[1-4]. After a general introduction to the theory of spin relaxation and decoherence in solid state, we will address its detailed application for spin-½ molecules exhibiting room temperature coherence[1-3]. Results will encompass the most recent developments, including unpublished material, and an overlook to future development directions.

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In-situ EPR applied for speciation of active metal sites in zeolites

Susanne Mossin[1], Qi Gao[1], Thomas K. Rønne-Nielsen[1], David Nielsen[1], Ton V. W. Janssens[2] and Peter N. R. Vennestrøm[2,3]

[1] Department of Chemistry, Technical University of Denmark, 2800 Kgs., Lyngby, Denmark; [2] Umicore Denmark, 2970 Hørsholm, Denmark; [3] present association Topsoe A/S, Denmark

slmo@kemi.dtu.dk

EPR is a powerful quantitative spectroscopic method for following catalytic processes. It can be applied for heterogeneous transition metal catalysts even at realistic temperatures (150-300 °C).

Copper centers in zeolites are active catalysts in the selective catalytic reduction (SCR) of NO(g) and NO_2(g) with NH_3. The catalytic poison SO_2 deactivates the catalyst but the activity partially recovers after thermal regeneration. The reason for the permanent deactivation is disputed.

In-situ EPR protocols are applied to copper chabazite (Cu-CHA) zeolite catalyst materials with different amounts of copper. First, we show how the alumina distribution in the zeolite affects the copper speciation and reconcile the quantifications performed by hydrogen temperature programmed reduction and by in-situ EPR on the same material series.[1,2]

Second, we show the EPR can be used to reveal the reason for permanent catalyst deactivation by gas phase SO_2 exposure. The differences between fresh, SO_2-poisoned and regenerated catalysts are revealed by identifying and quantifying the copper sites and the time resolved speciation of Cu sites during reduction and oxidation half cycles (Fig. 1).[3]

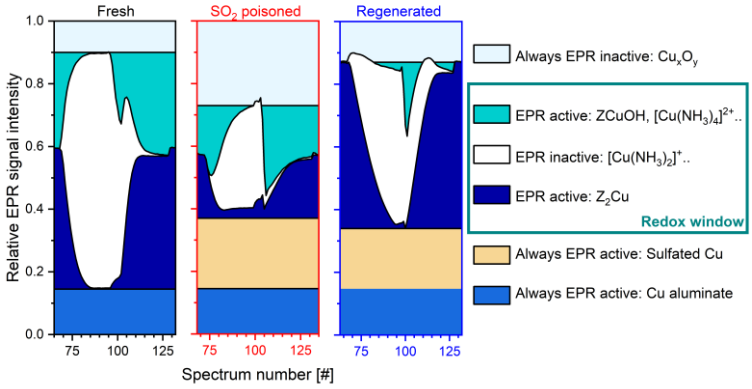

Figure 1. Cu species distribution determined by in-situ EPR protocols at 200°C during reduction (spectrum # 70-100, in 1000 ppm of NO+NH_3) and then oxidation (spectrum # 100-125, in 1000 ppm NO + 10 % O_2) of Fresh, SO_2-poisoned and Regenerated Cu-CHA (Si/Al = 7, 4.0 wt.% Cu).

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CONTRIBUTING TALKS

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Graphene Quantum Dots as Single-Molecule-Magnet detectors

Paola Barbara,[1] Amjad Alqahtani,[1] DaVonne Henry,[1] Lubomir Havlicek,[2] Luke St. Marie,[1] Jakub Hruby,[3] Antonin Sojka,[2] Morgan Hale,[4] Samuel Felsenfeld,[5] Abdellouahed El Fatimy,[6] Rachael L. Myers-Ward,[7] D. Kurt Gaskill,[5] Ivan Nemec,[8] Petr Neugebauer,[2] Amy Y. Liu[1]

[1] Georgetown University, Washington DC, USA; [2] CEITEC BUT, Czech Republic; [3] National High Magnetic Field Laboratory, Tallahassee, FL, USA; [4] Roanoke College, VA, USA; [5] University of Maryland, College Park, MD, USA; [6] Mohammed VI Polytechnic University, Morocco; [7] Naval Research Laboratory, USA; [8] Palacky University Olomuc, Czech Republic.

Paola.Barbara@georgetown.edu

The thermally-activated electrical current channel in graphene nanoconstrictions yields sensitive detection in a wide temperature range.[1] Here we describe our work using quantum dots patterned from epitaxial graphene on SiC as detectors for electron paramagnetic resonance [2] and as detectors for magnetization switching of single molecule magnets,[3] for the archetypal Mn_{12}. The use of epitaxial graphene on a substrate that is CMOS compatible provides a route for scalable applications.

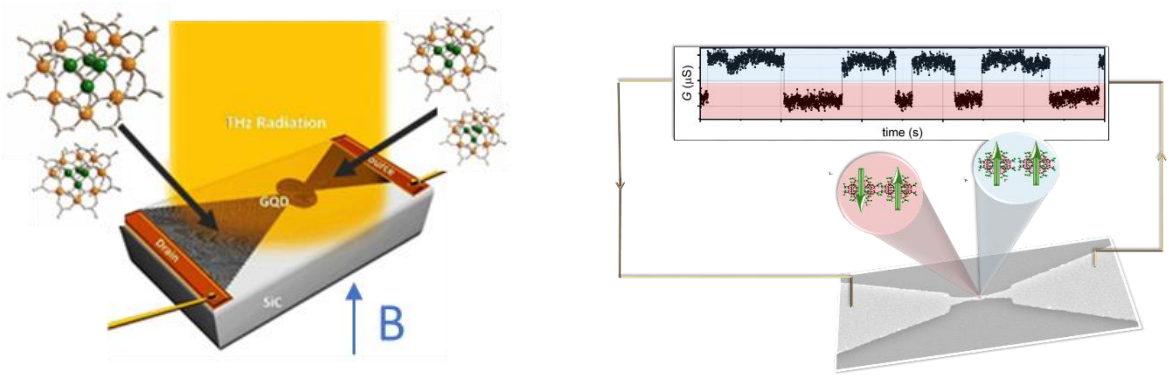

Figure 1: Schematic of graphene quantum dots as EPR detectors (left) and detectors of SMM magnetization switching (right).

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NMR and EPR Integration Uncovers Dynamic Architecture of Human Chaperone DNAJB1

Yasmin Ben-Ishay,[1] Michael Maurer,[1] Oran Melanker[1] and Rina Rosenzweig[1].

[1]Department of Structural Biology, Weizmann Institute of Science, Rehovot, Israel

Yasmin.Ben-Ishay@weizmann.ac.il

J-domain proteins (JDPs, Hsp40s) tightly regulate the ATP-driven activity of heat shock protein 70 (Hsp70), a key component of cellular proteostasis. JDPs interact with Hsp70 via a conserved J-domain that stimulates ATP hydrolysis and substrate processing. The human JDP family comprises over 50 members divided into four subclasses, however, class B JDPs exhibit a distinct regulatory mechanism. In DNAJB1, a unique GF-rich α-helix (Helix V) docks onto the J-domain, blocking Hsp70 interaction.[1] This autoinhibition is relieved when the Hsp70 C-terminal EEVD motif binds the CTDI domain, distal to the J-domain, revealing a long-range allosteric mechanism. The structural basis of this regulation remains unresolved, largely due to the absence of a high-resolution full-length structure of DNAJB1, as its conformational flexibility has hindered characterization by conventional structural approaches.

Here, we combine site-directed spin labeling with high-resolution paramagnetic relaxation enhancement (PRE) and double electron–electron resonance (DEER) spectroscopy to probe the dynamic architecture of full-length human DNAJB1 chaperon (Figure 1). This integrative paramagnetic approach provides new insights into the structural organization of DNAJB1 and offers a framework for elucidating how binding of the Hsp70 EEVD motif may trigger the release of Helix V from the J-domain, thereby regulating Hsp70 activation. These insights will advance our understanding of Hsp70 regulation and its role in amyloid disaggregation, with potential implications for therapeutic strategies targeting protein aggregation in neurodegenerative disease.

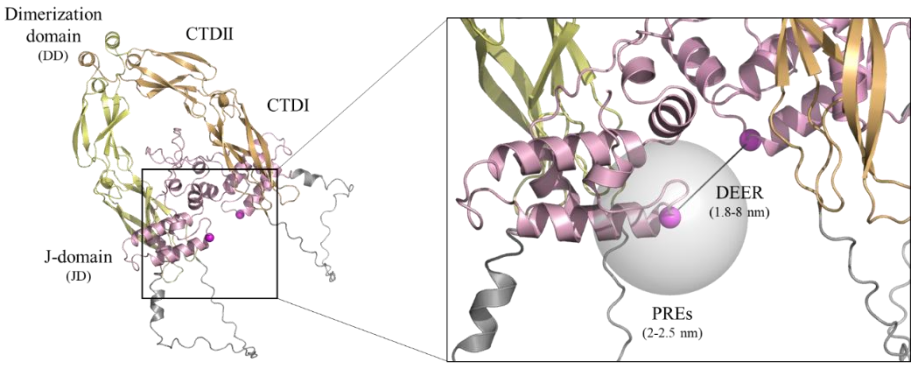

Figure 1: Deciphering the dynamic structure of DNAJB1 at atomic resolution using paramagnetic resonance spectroscopy (PREs and DEER).

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New Application-Specific ESR Resonators

Aharon Blank

Tel-Aviv University, School of Electrical and Computer Engineering, Israel; Schulich Faculty of Chemistry, Technion – Israel Institute of Technology

ab359@tau.ac.il

Roughly speaking, ESR instruments are all alike: they consist of a magnet, a spectrometer, a microwave bridge, and operating software. While the details differ between systems, the underlying principles are largely the same. In many cases, however, what makes an ESR system unique, specialized, and more effective for a given application is the **microwave resonator**. The microwave resonator is where "all the action" occurs. For standard tube-like samples, there are many commercially available resonators that perform adequately. However, in many applications involving unconventional sample geometries or compositions, conventional resonators either perform poorly or cannot be used at all. In such cases, one must resort to **custom-designed resonators** optimized for the specific sample, the specific application, or both. Our laboratory develops such specialized resonators. For example, we have recently developed a **dual-frequency dielectric resonator** that can be used to excite and receive signals at X-band at two distinct frequencies separated by ~2.87 GHz. This is particularly useful for experiments where both **NV centers in diamond** and standard $g \approx 2$ spins need to be addressed and/or detected. Another example is a **2D microstrip-based resonator** designed for acquiring high signal from flat, planar samples (Figure 1). We have also developed a **miniature loop-gap resonator** that can be tuned over the ~2–8 GHz range, suitable for measuring lossy samples or **optically detected ESR** samples. In addition, we have designed resonator structures for supporting **diamond-based maser activity**, featuring optical illumination ability, high quality factor (Q) and extremely high filling factor. These and additional unconventional resonator structures will be presented in the talk, along with their design principles, simulation results, and measured performance.

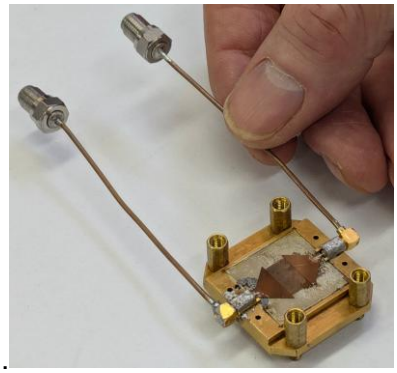

Figure 1: Surface resonator for 2D samples with dual in/out ports.

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Investigating Protein Structure and Function *in Vitro* and in Cells Through Copper(II) Spin-Labelling

Katrin Ackermann, Yannik Limbach, Aisika Chakraborty, Bela E. Bode

EaStCHEM School of Chemistry, Biomedical Sciences Research Complex and Centre of Magnetic Resonance, University of St Andrews

beb2@st-andrews.ac.uk

EPR Spectroscopy is a method of choice for investigating the binding sites of paramagnetic metal ions in proteins. However, recent reports show that artificially introduced *cis*-double histidine (dHis) sites are an excellent avenue for high sensitivity application of pulse dipolar EPR spectroscopy (PDS) *in vitro*[1] and even in cells.[2]

In this contribution we will demonstrate how PDS allows identifying binding sites and their occupation in serum albumin,[3] an important transporter of fatty acids, Zn^{II} and other cofactors in mammalian blood that are implicated in diabetes, obesity and further medical conditions.

Furthermore, engineering dHis sites into proteins allows distance measurements at sub-micromolar concentrations and within cells. The success of these experiments crucially depends on binding site affinity, and we will demonstrate the mechanisms underpinning this.[4]

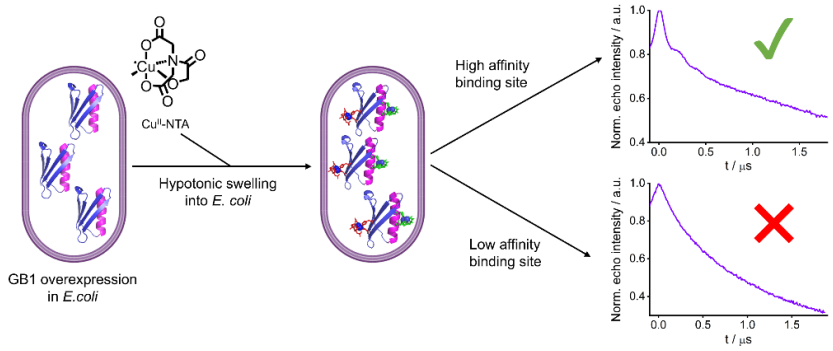

Figure 1: Cartoon illustrating in-cell EPR success depending on binding site affinity.

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Orientation of the Zero-Field Splitting Tensor in Gd(III) Chelates Probed by Orientationally Selective ENDOR

Alexey V. Bogdanov,[1,*] Veronica Frydman,[1] Manas Seal,[1,2] Wenkai Zhu,[3,4] Alexander Schnegg,[5] Angela M. Gronenborn,[3] Xun-Cheng Su,[6] Daniella Goldfarb[1]

[1] Weizmann Institute of Science, Rehovot 7610001, Israel; [2] Indian Institute of Technology, Kharagpur 721302, WB, India; [3] University of Pittsburgh, 4200 Fifth Ave, Pittsburgh, PA 15260, United States; [4] State Key Laboratory of Magnetic Resonance Spectroscopy and Imaging, National Center for Magnetic Resonance, Chinese Academy of Sciences, Wuhan, 430071 P. R. China; [5] Max Planck Institute for Chemical Energy Conversion, 34-36 Stiftstraße, Mülheim an der Ruhr, 45470, Germany; [6] Nankai University, Tianjin 300071 P. R. China.

alexey.bogdanov@weizmann.ac.il

The zero-field splitting (ZFS) interaction governs the electron spin energy level structure and relaxation behavior of Gd(III) complexes and is therefore central to their performance in EPR spectroscopy and as spin labels. While the magnitude of the ZFS is routinely estimated, its orientation in the molecular frame remains largely inaccessible experimentally for Gd(III) chelates in frozen solution. This limitation hampers quantitative analysis of anisotropic interactions and restricts the accuracy of structural and dynamical interpretations in Gd-based EPR methodologies.

We present an experimental approach for direct determination of the ZFS tensor orientation in Gd(III) complexes. Using a series of fluorinated Gd(III) chelates, we exploit orientation-selective ^{19}F ENDOR measurements on high-$|m_S|$ electron spin transitions, where sensitivity to the ZFS principal axes is maximized. By combining ENDOR data from multiple fluorinated derivatives of the same chelate, we determine the orientations of the principal axes of the ZFS tensor in the molecular frame (Fig. 1).

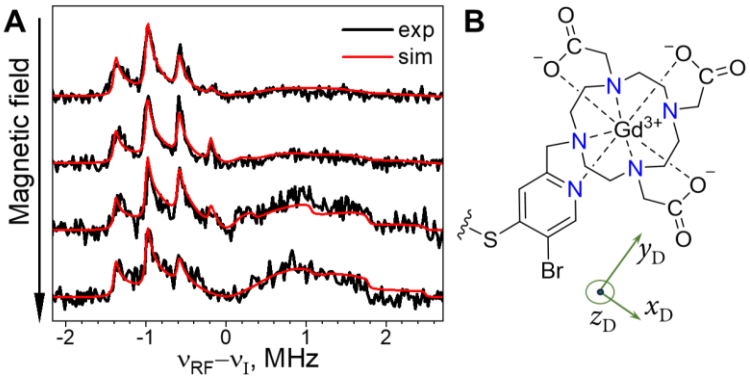

Figure 1: (A) Experimental (black) and simulated (gray) magnetic field dependence of ^{19}F ENDOR spectra of a Gd-DO3A complex featuring orientation selection and (B) the scheme showing the principal axes of Gd(III) ZFS in the corresponding chelate, experimentally determined from the spectra of a set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

Knowledge of the ZFS orientation enables a consistent treatment of anisotropic electron–nuclear interactions in Gd(III) systems. It allows separation of distance and angular contributions in Gd–F couplings and improves the interpretation of orientation-selective ENDOR spectra. We illustrate how this information can be leveraged to extract orientational constraints in Gd- and fluorine labeled proteins.

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Unusual Positive Fermi Contact Interaction for Square-Planar Copper Complex revealed by TRIPLE ENDOR experiments

Paolo Cleto Bruzzese,[1,2] Haowei Chen,[3] Yang Liu,[4] Franc Meyer,[5] Alexander Schnegg[2] and Shengfa Ye[6]

[1] Department of Chemistry, University of Turin, Turin, Italy; [2] Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany; [3] Max Planck Institute for Coal Research, Mülheim an der Ruhr, Germany; [4] Institute of Inorganic Chemistry, University of Regensburg, Regensburg, Germany; [5] Institute of Inorganic Chemistry, Georg-August-University Göttingen, Göttingen, Germany; [6] Key Laboratory of Bioinorganic and Synthetic Chemistry of Ministry of Education, Sun Yat-sen University, Guangzhou, China.

paolocleto.bruzzese@unito.it

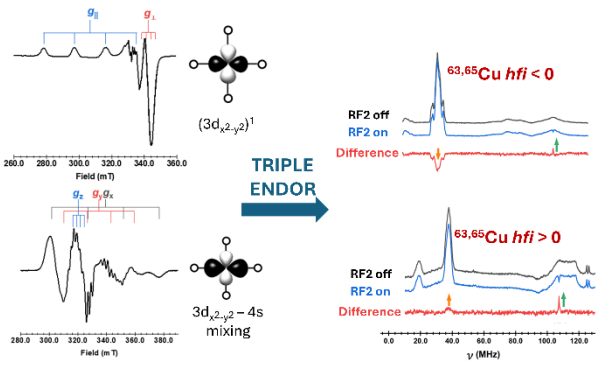

Figure 2. Schematic diagram of ligand-induced d-s mixing in Cu(II) and their influence on the EPR spectra

Paramagnetic copper(II) species are widespread in catalysis, material science, bioinorganic and medicinal chemistry.[1] Determining the structural and electronic parameters that dictate the coordination behaviour of Cu(II) complexes is essential to connect molecular architecture with reactivity and, eventually, engineer novel copper-centered systems. EPR and related hyperfine techniques are well suited to probe Cu(II) species and to correlate spectroscopic parameters with molecular geometry and electronic structure.[2]

The vast majority of Cu(II) complexes adopts square-planar geometry, readily identified by the EPR fingerprint $g_\parallel > g_\perp \approx 2.0023$ and $|^{Cu}A_\parallel| >> |^{Cu}A_\perp|$. Here, we investigate a square-planar Cu(II) complex displaying a reversed copper hyperfine anisotropy $|^{Cu}A_\parallel| \ll |^{Cu}A_\perp|$, while retaining the usual **g**-tensor pattern. TRIPLE ENDOR experiments reveal that the copper hyperfine coupling has a positive sign – contrary to the commonly observed negative sign – accounting for the unusual hyperfine pattern (Figure 1). Ab-initio calculations suggest that the positive sign results from strong 4s mixing in the ground state caused by the ligand scaffold's donor strength. The results highlight the sign of the copper hyperfine coupling as a sensitive magneto-structural probe that expands the established framework for Cu(II)-based complexes.

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Insights into the High-Spin S_2 State in Photosynthetic Water Splitting

Maria Chrysina [1,2]

[1] Institute of Nanoscience & Nanotechnology, NCSR "Demokritos", Athens, Greece; [2] Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany

m.chrysina@inn.demokritos.gr

Photosystem II utilises sunlight to drive the four-electron oxidation of H_2O to O_2. This reaction occurs at a $Mn_4CaO_{5/6}$ cluster, which cycles through five oxidation states, S_0-S_4. The $S_2 \rightarrow S_3$ transition - the last step before O_2 formation - is a multistep process involving deprotonation, oxidation, and water binding. The sequence of events and the nature of possible intermediates remain controversial, partly because multiple forms exist in the S_2 state ($Mn^{III}Mn^{IV}_3$), and it is unclear which one progresses to S_3. The S_2 configurations are distinguished only by their EPR signals. The dominant S = 1/2 S_2 form gives rise to the well-known g ≈ 2 "multiline" signal, commonly accepted to contain a Mn^{III} with an empty coordination site that could accept a water ligand. A $g \approx 5$ (possibly S = 7/2) S_2 configuration has been proposed as an intermediate between S_2 and S_3 (Mn^{IV}_4), possibly representing a water-bound S_2 state [1]. Despite its functional significance, the structural and electronic properties of the $g \approx 5$ form remain unknown, making its characterisation crucial for unravelling the mechanistic details of the $S_2 \rightarrow S_3$ and, in particular, the water-binding step. In this study, the high-spin S_2 state ($g \approx 5$) of *T. vestitus* was investigated using X and W-band EPR spectroscopy, including electron-electron double resonance (ELDOR) detected NMR (EDNMR). The results are discussed in the context of proposed structural models for the high-spin S_2 configurations.

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Detection of Spin-Electric Effects in Spin Triangles by Electric Field Modulated EPR Spectroscopy

Alberto Cini,[1] Leonardo Passerini[1,2], Idris Tlemsani[2], Valerio Briganti[2], Daniele Sartini[2], Shubham Bisht[3], Benjamin Kintzel[4], Michael Böhme[4], Winfried Plass[4], Federico Totti[2], Michael Shatruk[3], Maria Fittipaldi[1], Roberta Sessoli[2]

[1] Department of Physics and Astronomy and INSTM Research Unit, University of Florence, via Sansone 1, I-50019, Sesto Fiorentino, Italy; [2] Department of Chemistry 'Ugo Schiff' and INSTM Research Unit, University of Florence, via della lastruccia 3-13, I-50019 Sesto Fiorentino, Italy; [3] Department of Chemistry, Florida State University - FL 32306 Tallahassee, United States; [4] Institute of Inorganic and Analytical Chemistry, Friedrich Schiller University Jena, Humboldtstr. 8, 07743 Jena, Germany.

alberto.cini@unifi.it

Among magnetoelectric materials, those exhibiting spin-electric (SE) effects are gaining a growing interest, as the SE effect allows for the electric control of spins. Quantum information technology is expected to benefit from its achievement enabling a faster, energetically more convenient and more space-confined spin manipulation with respect to the standard approach based on the magnetic field.
The Electric Field Modulated Electron Paramagnetic Resonance (EFM-EPR), a technique recently implemented by some of us [1], which allows performing single-crystal EPR under an electric field, has been proven to be very effective for the detection of the SE effect, enabling also to address the possible anisotropy of the effect [2-4].
EFM-EPR data and comprehensive *ab initio* and DFT calculations allowed an in depth investigation of the SE effect on the $[Cu_3(saltag)(py)_6]ClO_4$ trimer [5], an antiferromagnetically coupled spin triangle evidencing no antisymmetric exchange Dzyaloshinskii-Moriya (DM) interaction. We demonstrated that when the electric field is applied in the plane of the triangle, the dominant contribution to the observed SE signal arises from a variation of the isotropic exchange interaction.
Recently, a strong SE effect was detected in the $[Cu_3(pz)(Im)_3(\mu_3\text{-}OH)(\mu_3\text{-}NO)(NO)]$ trimer [6], characterized by a sizeable DM interaction. The molecule has an isosceles geometry, leading to inequivalent isotropic Heisenberg exchange interactions between copper ion pairs. The experimental results are analyzed using computational modelling and complemented by magnetometry measurements to obtain a complete determination of the spin Hamiltonian parameters and to shed light on the microscopic origin of the SE effect and therefore on the mechanisms governing it.

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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]

[1] Department of Chemistry, Photon Science Institute and The National Research Facility for Electron Paramagnetic Resonance, University of Manchester, Manchester, UK; [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

susanna.ciuti@manchester.ac.uk

{Cr_7Ni} antiferromagnetically coupled rings (Figure 1a) have been proposed as potential molecular qubits, as two-level systems with agreeable phase memory times for gate operations[1] and flexibility for building multi-qubit systems.[2] To work towards the application of light-switchable molecular quantum gates, we present an investigation of different Cr-Ni systems via Time-resolved Electron Paramagnetic Resonance spectroscopy (trEPR) experiments. We observe, for the first time in these systems, strong, long-lived emissive trEPR signal (Figure 1b) and we interpret this 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.

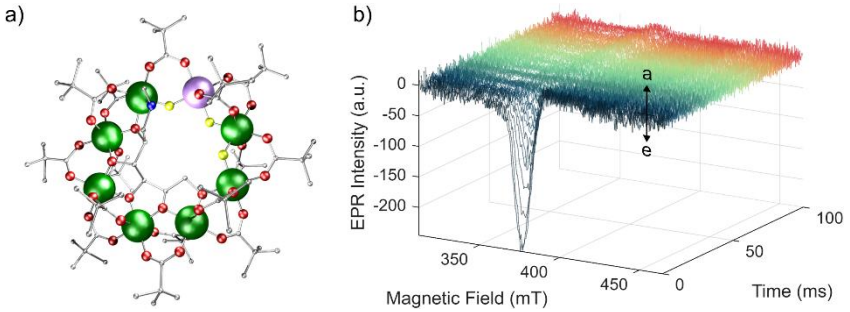

Figure 1: a) Crystal structure and b) trEPR spectrum at 3 K of a {Cr_7Ni} ring in a toluene:dichloromethane frozen solution, after excitation at 560 nm over time.

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Pulsed EPR and DNP at 94 GHz

Thierry Dubroca,[1] C. Korrigan Amadi,[1] Ilya Litvak[1]

[1] National High Magnetic Field Laboratory, Tallahassee, Florida USA

dubroca@magnet.fsu.edu

The National High Magnetic Field Laboratory (Maglab) in Tallahassee, Florida, acquired a High-Power EPR spectrometer (HiPER) in 2010, that is, a duplicate of the original instrument developed at the University of St. Andrew by the group of Graham Smith [1]. HiPER is based on a high-power microwave amplifier (1 kW) operating at 94 GHz with a Quasi-Optical system enabling the utmost EPR sensitivity at high magnetic fields. To make the most out of this very high sensitivity advantage, the Maglab HiPER is being upgraded with a variety of new elements (software and hardware) to enable advanced EPR and DNP experiments. An Arbitrary Waveform Generator (AWG) which, combined with NMR detection, enables pulsed DNP. The AWG also enables T_1 measurements without spin diffusion artefacts, measures fast spin diffusion and combined with a new 10 W solid state amplifier it permits the measurements of long relaxation times. We present here newly installed capabilities as well as upcoming developments. Overall, these recent upgrades have led to several publications with different collaborating groups [2-6].

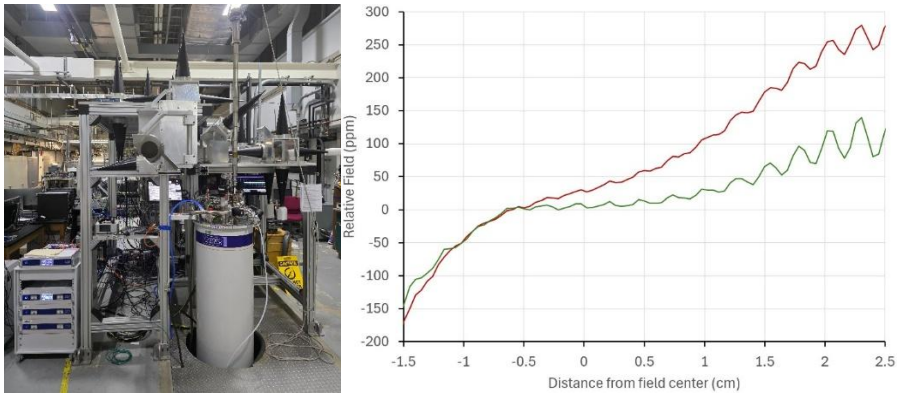

Figure 1: left: Picture of the recently upgraded Maglab HiPER spectrometer. Right: Magnetic field map at 3.4 T (as-is above in red, with ferroshims correction below in green).

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FRASCAN II: A Modular EPR/NMR/DNP Extension for NMR Systems

Jan Dubský,[1] Oleksii Laguta,[1] Petr Drexler, [2] Lucie Kotásková,[1] Ladislav Křenek,[3] Andriy Marko,[1] Thierry Dubroca,[4] Radovan Fiala,[5] Pavel Kadeřávek,[5] Petr Neugebauer,[1]

[1] Central European Institute of Technology, Brno University of Technology, Brno, Czech Republic; [2] Faculty of Electrical Engineering and Communication, Brno University of Technology, Brno, Czech Republic; [3] Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic. [4] National High Magnetic Field Laboratory, Tallahassee, Florida, USA; [5] Central European Institute of Technology, Masaryk University, Brno, Czech Republic.

Jan.Dubsky@ceitec.vutbr.cz

High-field EPR and dynamic nuclear polarization (DNP) remain largely confined to dedicated, costly instruments inaccessible to most NMR laboratories. Even where DNP is available, polarizing agents are typically characterized on a separate EPR spectrometer under different conditions, introducing systematic uncertainties when transferred to the DNP experiment.
We present FRASCAN II, a 329 GHz / 500 MHz EPR/NMR/DNP spectrometer built as a non-invasive, modular add-on to existing high-field NMR magnets. The current prototype operates on a Bruker Avance Neo 500 at 11.75 T, with the architecture transferable in principle to any commercial NMR system. Installation takes approximately 30 minutes, and standard NMR operation is restored immediately after removal.
The system comprises a custom EPR console, a quasi-optical EPR bridge driven by a low-power (~60 mW) solid-state microwave source,[1] and a home-built EPR/NMR/DNP probe whose modular electronics can be adjusted to cover a wide range of NMR-active nuclei. This single instrument performs Continuous Wave EPR, Rapid Scan EPR,[2] NMR, and DNP on the same sample (liquid or solid phase) at room temperature, using standard NMR/EPR tubes compatible with the Bruker SampleCase pneumatic sample feeder.
We showcase representative measurements across these modes, demonstrating that FRASCAN II brings high-field EPR and DNP onto existing NMR infrastructure at a fraction of the cost of gyrotron-based systems, providing a unified platform for in-situ characterization of polarizing agents and other molecular systems.

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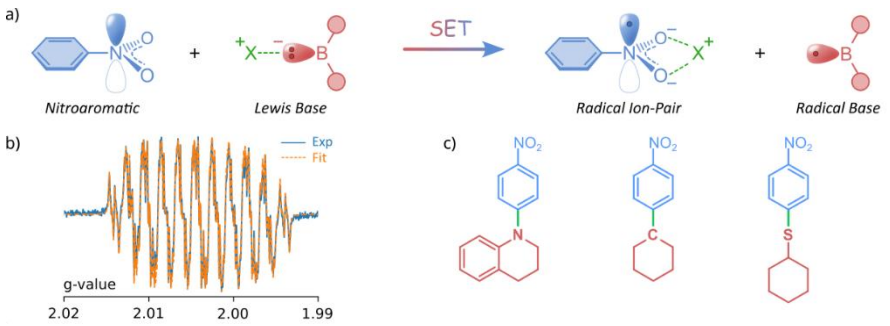
Exploiting SET-induced radical formation in organic synthesis

L. Ebo[1], S. Balahoju[2], J. Marvizón Valera[1], I. Zubillaga Nogueira[1], N. Bhattacharjee[2], L. Lezama[3], D. Reta[12]

[1] 1Department of Polymers and Advanced Materials, Faculty of Chemistry, The University of the Basque Country, UPV/EHU, Paseo Manuel Lardizabal 3, Donostia 20018, Euskadi, Spain; [2] 2Donostia International Physics Centre (DIPC), Paseo Manuel Lardizabal 4, Donostia 20018, Euskadi, Spain; [3] 3Inorganic Chemistry, University of the Basque Country, Barrio Sarriena, s/n, 48940 Leioa, Bizkaia, Spain

lisa.ebo@ehu

Knowledge of radical electronic structures enables the control of their properties and opens the potential of fine controlling their reactivity. Therefore, EPR is an unmatched technique, needed for the electronic structure characterization of organic radicals. However, the reactive nature of radicals and non-trivial preparational requirements limit the number of usable radical species until now. Enabling the generation of radical species under simple reaction conditions, employing available and inexpensive reactants, is therefore the key component for harnessing the extraordinary properties of organic radicals. Combining continuous wave (cw) X-band EPR spectroscopy, quantum chemical calculations, and synthesis, we demonstrate that this SET-induced mechanism operates across a broad set of commonly used nitroaromatic compounds, including FDA-approved drugs – these findings suggest a previously overlooked prevalence of nitroaromatic radical species. We further show how this framework resolves contested reaction mechanisms[4] and enables the rational exploitation of SET-derived radical pairs to access C-X (X=N, C, S) functionalization of nitroaromatic compounds regioselectily and in mild conditions. The understanding of the electronic structures of these radical pairs enables the utilization of radical compounds as reacting agents under mild synthetic conditions, laying the foundation for a new class of distinctive reaction mechanisms and thus unexplored opportunities in organic synthesis.



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Simulation tools for shaped-pulse control of molecular spins in pulsed EPR

Jean-Gabriel Hartmann,[1] Athanassios Boudalis,[1]

[1] Institut de Chimie, Université de Strasbourg, FR-67000 Strasbourg

jg.hartmann@unistra.fr

Molecular spin systems provide a versatile platform for developing control strategies in pulsed electron paramagnetic resonance (EPR). Shaped microwave pulses have enabled increasingly sophisticated manipulations of single- and coupled-spin states, with recent applications in quantum information processing methods [1,2] and feedback-based pulse-shaping optimisation [3]. However, reliable control of spin systems remains limited by experimentally relevant effects including hardware constraints such as finite bandwidth and pulse distortions, and sample-dependent effects such as ensemble broadening, as well as environmental interactions [4,5].

In this work, we present a pulsed-EPR simulation framework for modelling shaped-pulse control of molecular spin ensembles under experimentally realistic conditions. Several software packages are already well established for simulating, and analysing magnetic resonance experiments, but they often target different aspects of the problem. Building on the extensive functionality of EasySpin [6], the framework implements numerical tools for modelling complex shaped-pulse EPR sequences together with ensemble and environmental effects using an open quantum systems formalism.

We benchmark this framework using canonical pulsed-EPR experiments, including single-pulse FID and field-swept simulations, two-pulse echo, CPMG-like multi-pulse sequences, and long-nutation PEANUT experiments. The simulation results reproduce expected experimental trends, validating the framework as a basis for designing and assessing shaped pulses under realistic conditions. This provides a route towards integrating optimal control methods such as gradient ascent pulse engineering (GRAPE) [7] for robust, high-fidelity operations using arbitrary pulse shapes.

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Pulsed, Magic Angle Spinning EPR at 7 and 14 Tesla

Ilia Kaminker[1]

[1] School of Chemistry, Tel-Aviv University, Tel-Aviv, Israel

iliakam@tauex.tau.ac.il

High-field EPR is essential for an in-depth understanding of Dynamic Nuclear Polarization (DNP) – a prominent technique for signal enhancement in contemporary NMR. DNP is based on polarization transfer from an unpaired electron spin to neighboring nuclear spins. Since DNP performance depends on experimental conditions, typical low-field static EPR experiments are of limited relevance for studying modern, high-field Magic Angle Spinning (MAS) DNP, which requires the development of high-field pulsed MAS-EPR instrumentation and methodology. Recently, we reported the first high-field (7 T) pulsed MAS-EPR experiments at spinning rates up to 3 kHz [1].

In this work, we demonstrate MAS EPR experiments at spinning speeds up to 37 kHz and magnetic fields up to 14 T, including rotor-synchronized stimulated-echo MAS-EPR experiments, which allow observation of electron spin dynamics on the hundreds-of-microsecond timescale, an essential timescale for DNP investigations. Beyond investigating the DNP mechanism, we demonstrate the unique capability of MAS-EPR to separate EPR spectra by anisotropy.

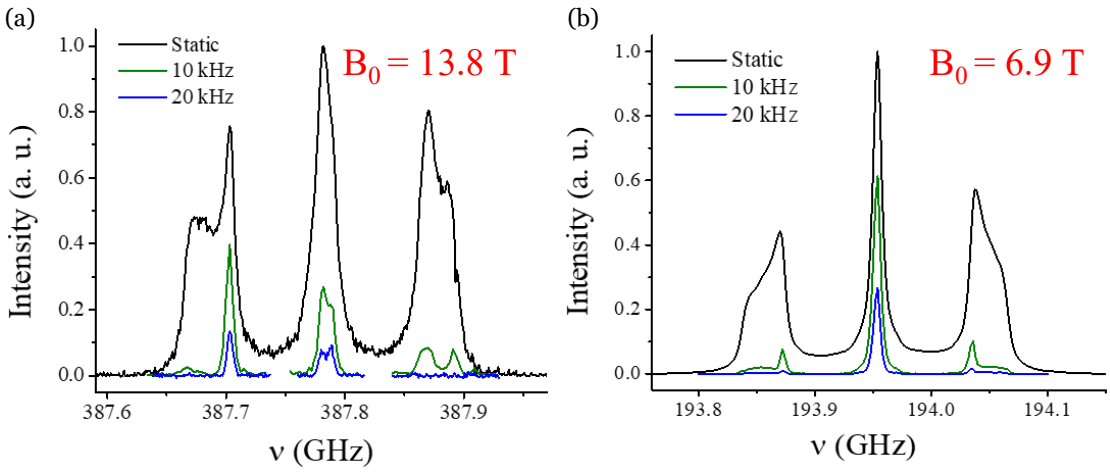

Figure 1: Changes in the 2-pulse EPR spectra of P1 centers in diamonds as function of the MAS frequency at 14 T (a) and 7 T (b).

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An Open Design Modular Ka Band Spectrometer

Hugo Karas,[1,2] Daniel Klose[1], Rene Tschaggelar[1], Enrica Bordignon[2], Gunnar Jeschke[1]

[1] ETH Zürich, Institute of Molecular Physical Science, 8093 ZH, Switzerland; [2] Department of Physical Chemistry, Sciences II, University of Geneva, 1211 Geneva, Switzerland;

hkaras@ethz.ch

We present a design for an open-source Ka-Band EPR pulse spectrometer that leverages the latest advances in 5G and satellite communication at a fraction of the cost of a comparable commercial instrument. Two spectrometers have been built from the design: First new life was brought to an old magnet at ETH; second, a completely new spectrometer was built at UNIGE using a state-of-the-art superconducting magnet.

Due to advances in arbitrary waveform generators (AWGs), pulse EPR spectrometer have become significantly simpler and easier to build. However, homebuilt spectrometers have remained mostly constrained to specialist hardware-focused research groups. We hope that through an open-modular design, like what we present here, more research groups will be able to benefit from homebuilt instrumentation and the latest developments in digital and microwave electronics.

The design has been optimised to minimise the necessary cost, whilst not sacrificing performance. Instead of a high-power TWT we have used a very affordable 40W (30-31 GHz) solid-state power amplifier (SSPA). Nonetheless we are still able to achieve a high B1 field (ν_1 = 60 MHz, Q=150) in a 1.6mm loop-gap resonator [1]. Further work is being done to evaluate using two 40W amplifiers in parallel to achieve sufficiently high B1 powers in a 3mm oversized-sample resonator [2], to boost the concentration sensitivity, ideal for DEER spectroscopy.

The spectrometer is controlled by an open-source Python-based modular control software with an easy-to-understand Python-based pulse programming language. An API allows for easy connection to software such as autoDEER [3], and a graphical user interface (GUI) shows key spectrometer parameters and the current measurement. The modular design allows for individual components to be replaced depending on the necessary specification (such as using a 34-36 GHz TWT) or as new better, cheaper components become available.

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Determination of local spin concentrations from instantaneous diffusion

Annemarie Kehl,[1] Olga Vojtiskova,[1] Gunnar Jeschke[1]

[1] Institute of Molecular Physical Science, D-CHAB, ETH Zurich

annemarie.kehl@phys.chem.ethz.ch

Commonly, EPR spectroscopy is applied to identify structural parameters on biomolecules for example by measuring distance distributions between two spin labels in a protein. However, in all EPR experiments the signal intensity is affected by decoherence properties leading to a background decay function if a time dependent signal is acquired. The decoherence properties are strongly dependent on the local environment. This includes the solvent that is surrounding the electron spin, the presence of methyl groups in the vicinity, and the local spin concentration. Determination of the latter is especially desirable in systems where differences in the local concentration occur, for example due to liquid-liquid phase separation. Decoherence properties can be directly measured using the sensitive Hahn echo decay experiment. Thus, this experiment can in principle be used to extract further information on the sample.

At low temperatures the main decoherence pathways are a spin bath dependent process and instantaneous diffusion. The spin bath process can be modelled by a stretched exponential decay and is dependent on the presence of methyl groups and the surrounding medium.[1,2] The instantaneous diffusion contribution depends on the local spin concentration and the flip angle of the second pulse (θ_2) in the Hahn echo decay sequence.[3] Here, we will show how the dependence on θ_2 can be used to identify local spin concentrations (Figure 1).

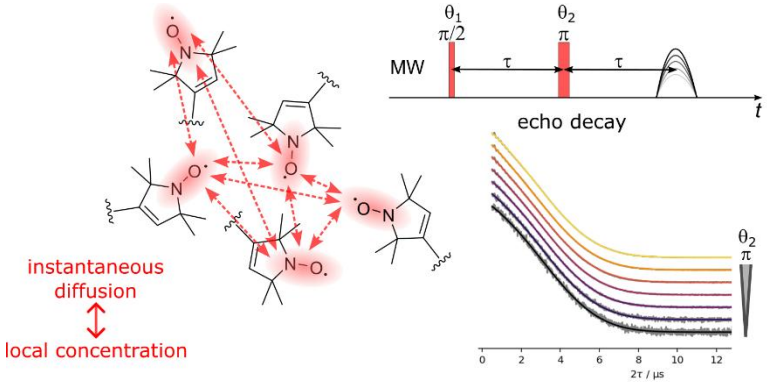

Figure 1: The instantaneous diffusion contribution to the Hahn echo decay can be separated from other contributions by varying the flip angle θ_2 which allows the extraction of local spin concentrations.

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EPR spectroscopy for a comprehensive analysis of functionalized magnetic nanostructures and their biological interactions

Tomasz Kubiak,[1] Bernadeta Dobosz[1]

[1] Faculty of Physics and Astronomy, Adam Mickiewicz University, Poznań, Poland

kubiakt@amu.edu.pl

Electron paramagnetic resonance (EPR) and ferromagnetic resonance (FMR) spectroscopy are invaluable tools in nanoparticle research. Extensive studies conducted by our group have demonstrated that EPR can play a pivotal role in characterizing nanostructures intended for theranostic applications and evaluating their biological interactions [1].
Our EPR spectroscopy and imaging experiments using magnetic core-shell nanoparticles with attached spin labels were performed using Bruker EMX-10 and Elexsys E540L spectrometers, operating at X-band (9.4 GHz) and L-band (1.1 GHz) frequencies, respectively.
The EPR/FMR investigation of spherical iron oxide nanoparticles of various sizes encompassed the identification of the core's material composition (magnetite, maghemite, or a combination of both), the assessment of changes in the Fe(II)/Fe(III) ratio in the crystal structure (maghemitization of magnetite grains due to aging), the characterization of the magnetization relaxation processes, the estimation of anisotropy constants and the examination of defects resulting from surface oxidation. In the case of nanoparticles coated with biocompatible polymer and labeled with 4-amino-TEMPO, in addition to the broad signal originating from the magnetic cores, the spectra also contained a characteristic triplet from nitroxide. Simulations performed using EasySpin toolbox allowed us to determine the parameters related to magnetic tensors and investigate the dynamics of the spin label in various media, including water, human serum and whole blood [2]. The anisotropy of the motion of spin label reflected its interactions with the surrounding medium and the manner of the attachment of the nitroxide to the surface of nanoparticles. Spin labels and EPR imaging technique enabled us to monitor the spreading kinetics of nanoparticles following their injection into tissue-mimicking phantoms [3]. EPR investigations of the interactions between TEMPO-labeled ferrite nanoparticles and the biological environment also included the mechanisms of their endocytosis into yeast cells and tracking their intracellular fate [4]. Moreover, we checked whether iron-containing nanoparticles can contribute to the generation of reactive oxygen species in tissues and to what extent the polymer coating reduces the risk of radical reactions. In order to detect short-lived radicals we used DMPO and DEPMPO spin traps. Our research proved that EPR/FMR techniques can significantly expand the knowledge of the properties and interactions of magnetic nanoparticles.

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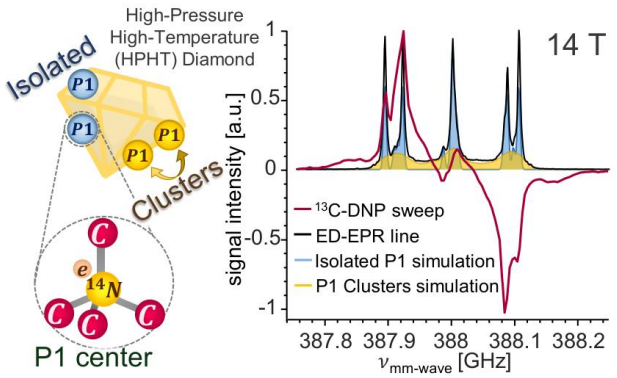
EPR at NMR Magnetic Fields: A New Perspective on P1-DNP in Diamond

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

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

oritnir1@mail.tau.ac.il

High-field EPR (HF-EPR) has been central to EPR method development, offering improved g-factor resolution, narrower spectral features in half-integer high-spin systems, and enhanced nuclear-frequency separation in ENDOR. More recently, it has become essential for understanding DNP mechanisms at the high magnetic fields used in modern NMR (≥ 7 T).



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

DNP enhances NMR sensitivity by transferring polarization from electron spins to nuclear spins and is typically performed at high magnetic fields to benefit from the increased NMR resolution. However, the mechanistic interpretation of DNP is often limited by the lack of corresponding HF-EPR measurements. This limitation is particularly evident in diamonds, where unexpectedly efficient ^{13}C-DNP has been observed from substitutional nitrogen, or P1, centers at magnetic fields up to 14 T, despite the expected suppression of the solid effect at these fields.[1–3]

We investigated this anomaly using our group's home-built dual DNP/EPR spectrometer operating at 7 and 14 T over 8–300 K.[4] The instrument enables CW and pulsed EPR, ELDOR, and multinuclear DNP measurements on the same sample under identical conditions. The HF-EPR enabled by this instrument reveals that the P1 spin system is more complex than inferred from low-field studies alone. Alongside isolated P1 centers, we identify a significant population of exchange- and dipolar-coupled P1 clusters, observed as a broad component underlying the canonical P1 EPR spectrum.[3] By combining pulsed EPR, ELDOR, and DNP, we showed that these coupled P1 clusters provide the electron-spin pairs required for cross-effect polarization transfer, explaining the efficient ^{13}C-DNP observed in HPHT diamonds.[5]

These results demonstrate that HF-EPR is indispensable for interpreting and optimizing DNP at NMR-relevant magnetic fields.

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When does a spin become a qubit? An EPR view at the molecular level

Valentin Novikov

Department of Inorganic Chemistry, University of Barcelona, Barcelona, Spain

novikov@ub.edu

In recent years, quantum information processing has become a major source of inspiration for the EPR community. Electron spins can, in principle, serve as elementary units of quantum computation, and molecular systems hosting such spins are often described as molecular qubits. Despite the considerable hype in this field, where almost any paramagnetic compound with transverse spin relaxation times long enough to allow pulsed EPR detection is sometimes labeled a molecular qubit, a growing number of EPR studies now focus on measuring relaxation times, reporting coherence metrics, and performing nutation experiments that are frequently interpreted in terms of quantum control.

At the same time, the relationship between these experiments and practical quantum computing remains far from straightforward. While pulsed EPR provides powerful tools to probe spin dynamics, the extent to which standard observables such as T1, Tm, or Rabi oscillations translate into meaningful quantum information functionality is still unclear. This raises a broader question: what is the actual role of EPR spectroscopy in the context of quantum technologies, and where does it genuinely provide unique and reliable insight?

In this talk, I will address this question from the perspective of molecular spin systems. Using chromium-based complexes as a model platform, I will discuss how supramolecular encapsulation[1] can be used not only to engineer spin relaxation properties, but also to disentangle different decoherence mechanisms. In particular, encapsulation strategies can either suppress coupling to lattice vibrations[2] or modify the electronic structure of the spin center, for example by promoting spin delocalization onto the ligand framework and enabling clock transitions.

These results illustrate that, regardless of the ultimate prospects of molecular spins in scalable quantum computing, EPR remains uniquely suited to investigate decoherence at the molecular level. Supramolecular approaches provide a chemically tunable route to control these processes and to identify regimes where genuinely nontrivial spin dynamics can be observed[3].

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Orientationally-resolved electron spin relaxation and coherence in rare-earth dimers with a single-electron metal-metal bond

Alexey A. Popov,[1] Michal Zalibera,[2] Fupin Liu,[1] Marco Rosenkranz,[1] Leonid Rapatskiy,[3] Alexander Schnegg[3]

[1] Leibniz Institute for Solid State and Materials Research Helmholtzstraße 20, 01069 Dresden, Germany; [2] Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic; [3] Max Planck Institute for Chemical Energy Conversion, Mülheim (Ruhr), Germany

a.popov@ifw-dresden.de

Encapsulation of magnetic species within robust molecular containers is a natural route towards stable and processable molecule magnets. Fullerenes provide an ideal platform for this goal since they are able to stabilize simple yet unconventional metallic species in their interior space and thereby. A spectacular example of this sort is the realization of the metal-metal bonding within the fullerene cage, which for a long time deemed not possible in conventional lanthanide chemistry. Particularly interesting are single-electron metal-metal bonds in dimetallofullerenes as the way to create very strong magnetic interactions between lanthanide magnetic moments,[1-3] or as the way to realize very strong hyperfine coupling due to the large s-orbital contribution to the M−M bonding orbital.[4,5] In this contribution we will overview CW and pulsed EPR studies of endohedral rare-earth dimers inside fullerene cages, with the main focus on spin distribution in Y_2 , Gd_2 and YGd dimers, their spin-lattice relaxation times and their relations to spin-phonon coupling.[6]

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Quantum sensing with spin defects in boron nitride nanotubes

Roberto Rizzato, PhD

Technical University of Munich, TUM School of Natural Sciences, Chemistry Department, Lichtenbergstraße 4,85748 Garching bei München

roberto.rizzato@tum.de

Optically addressable spin defects in wide-bandgap semiconductors have become a cornerstone of quantum sensing and metrology. While defects in bulk materials like diamond and silicon carbide have established the field, a new frontier is emerging with spin defects in boron nitride-based low-dimensional architectures that overcome the limitations of bulk technologies.
In my talk, I will focus on the exploration of novel spin defects in boron nitride nanotubes (BNNTs) [1,2] for nanoscale magnetic resonance sensing. These systems offer a unique combination of structural and quantum advantages: a naturally high surface area, hollow interiors for molecular confinement, and an omnidirectional spin response arising from optically active spin-½ defects [2, 3]. These features allow each nanotube, regardless of its orientation, to act as an active quantum sensor directly interfaced with its environment.
In our recent work, we demonstrated that the spin coherence times of these defects can be significantly extended, enabling advanced quantum-sensing protocols such as radio-frequency magnetometry with sub-hertz spectral resolution. These results anticipate future implementation of nanoscale NMR methods with these systems. Furthermore, when integrated into microfluidic environments, BNNT-based meshes operate as nanoporous sensors capable of detecting paramagnetic ions at micromolar concentrations, up to a thousand times lower than comparable hBN-based quantum sensors. This remarkable sensitivity likely arises from the nanotubular geometry, which maximizes analyte contact and confines molecular interactions within the sensing volume [2].
Altogether, these properties open promising avenues for nanoscale magnetic resonance spectroscopy using these systems.

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Detection of radicals in solution and at electrodes using spectro-electrochemical EPR-on-a-chip techniques

Takuma Sato,[1] Kaltum Abdiaziz,[1] Markus Teucher,[1] Silvio Künstner,[2] Anh Chu,[3]

Jens Anders,[3] Klaus Lips,[2] Alexander Schnegg[1]

[1] EPR research group, MPI-CEC, Mülheim an der Ruhr, Germany; [2] Berlin Joint EPR Laboratory and EPR4Energy, ASPIN, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany; [3] Institute of Smart Sensors, Universität Stuttgart, Stuttgart, Germany

takuma.sato@cec.mpg.de

Spectroelectrochemical-EPR (SEC-EPR) identifies paramagnetic specimen under variable electrochemical (EC) conditions. SEC-EPR set-ups must, on the one hand, meet the requirements of the electrochemical reaction – in particular, the ability to apply an external potential and ensure efficient mass transport in the solution – and, on the other hand, enable efficient microwave excitation. Here we compare two set-ups that follow different design criteria; On the one hand, SEC-EPRoC where an EPR-on-a-chip (EPRoC) sensor is immersed into the electrolyte of an electrochemical cell, and on the other, SEC-EPR where a miniaturised electrochemical cell is inserted into the sample tube of a benchtop EPR spectrometer (Figure 1a and b, respectively). We discuss the pros and cons of both set-ups and demonstrate how complementary time-resolved SEC-EPR and SEC-EPROC spectroscopy can be used to obtain quantitative information on radical formation at the electrode and in the bulk.

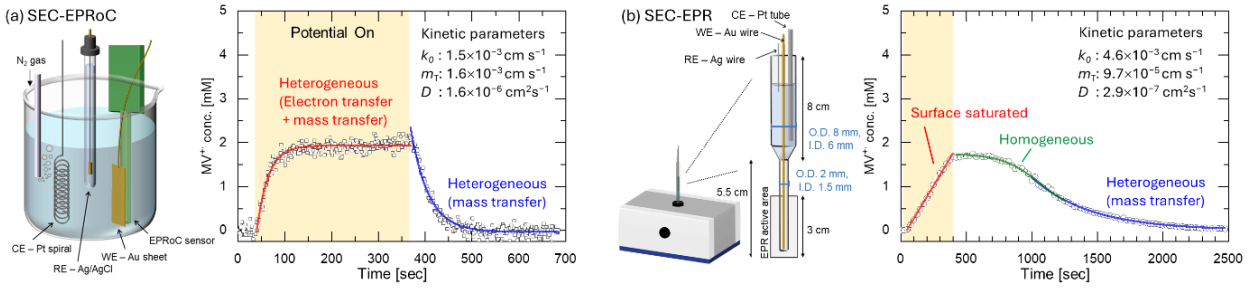

Figure 1: Schematic setup and temporal evolution of electrochemically generated $MV^{+\bullet}$ radical at potential of −0.57 V vs SHE for (a) SEC-EPRoC and (b) SEC-EPR, together with kinetic parameters in each setup.

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Terahertz Magnetic-Resonance Mueller Matrix Ellipsometry

Mathias Schubert,[1,2] Viktor Rindert,[1,2] Vanya Darakchieva[3]

[1] University of Nebraska-Lincoln, Lincoln, NE, 68511 USA; [2] NanoLund and Solid State Physics, Lund University, S-22100 Lund, Sweden; [3] Terahertz Materials Analysis Center and Center for III-Nitride Technology, C3NiT - Janzén, THeMAC, Lund University, S-22100 Lund, Sweden

schubert@engr.unl.edu

Terahertz (THz) magnetic resonance Mueller matrix Ellipsometry is a radical extension of magnetic-resonance spectroscopy by complete polarization-resolved measurement of the linear electromagnetic response of nuclear and electron spin associated magnetic resonance using far-field polarization optics at high magnetic fields.[1] Our new method evolves from the previously reported THz Optical Hall effect where, for example, measurements of free charge carriers under strong external magnetic fields provide access to critical band structure properties of semiconductors.[2] This new method permits us to accurately test existing models and leads to discovery of new physics in magnetic resonance such as the dynamic Bloch susceptibility model at THz frequencies,[3] the magnetic Lyddane-Sachs-Teller relationship,[4] the existence of longitudinal magnetic resonance modes,[4] the temperature-dependence of the Brillouin magnetization,[4] and rules of non-reciprocal sum and super convergence in dielectric, magnetic, and magnetoelectric spectral response dyadics. Our new method provides sensitive information about quantum properties of defect and dopants, demonstrated for key semiconductors such as SiC [1], Ga2O3 [5,6], and GaN [3,4] but will also be broadly applicable to magnetic and ferromagnetic resonances, and more.

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Development of time-domain ENDOR for electron-nuclear and nuclear-nuclear distance determination

Lucca Sielaff,[1,2] Sergei Kuzin,[1] Annemarie Kehl, [3] Karoline Goldschmidt, [2] Anakin Aden, [2] Andreas Meyer, [1,2] Marina Bennati, [1,2]

[1] Research Group EPR Spectroscopy, Max Planck Institute for Multidisciplinary Sciences, Am Faßberg 11, 37077 Göttingen, Germany [2] Institute of Physical Chemistry, Georg August University of Göttingen, Tammannstraße 6, 37077 Göttingen, Germany; [3] ETH Zürich, Department of Chemistry and Applied Biosciences, Vladimir-Prelog-Weg 1-5 / 10, 8093 Zürich, Switzerland

lucca.sielaff@mpinat.mpg.de

^{19}F electron–nuclear double resonance (ENDOR) has emerged as a powerful technique for probing electron–nuclear distance distributions in the 5–20 Å range. In contrast to NMR, most ENDOR experiments are still performed in the frequency-domain. In this approach, the full magnetic interaction of the ^{19}F spin contributes to the spectrum, resulting in ENDOR line widths of 10–30 kHz that limit the resolution. Here, we present time-domain ENDOR [1][2] experiments that substantially enhance the spectral resolution. Central to this approach is the coherent time evolution and manipulation of nuclear spins, which enables the disentanglement and quantification of individual nuclear spin interactions. Applied to model systems containing multiple fluorine nuclei, time-domain ENDOR experiments directly report on homonuclear and hyperfine couplings, which allows the extraction of associated electron-nuclear and nuclear-nuclear distance distributions (Figure 1). These results present time-domain ENDOR as a versatile platform for probing nuclear interactions, paving the way for new structural studies.

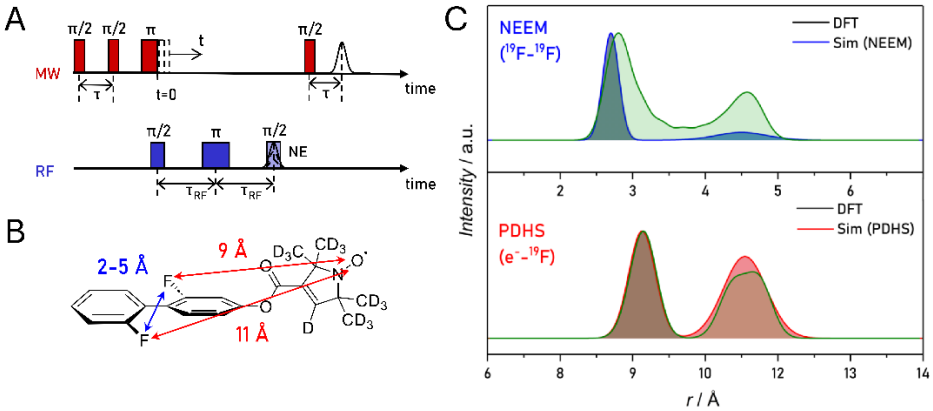

Figure 1: A) schematic time domain ENDOR pulse sequence. B) nitroxide model compound. C) Experimental distance distributions extracted from time domain ENDOR and DFT simulations.

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The origin of the asymmetry in spin-electric active antiferromagnetic equilateral triangles: an experimental and theoretical challenge

Lorenzo Sorace,[1] Daniele Sartini,[1] Jakob K. Staab,[1] Shubham Bisht,[2] Bijoy Nharangatt,[1] Federico Totti,[1] Michael Shatruk,[2] and Roberta Sessoli[1]

[1] Department of Chemistry "Ugo Schiff", University of Florence, 50019 Sesto Fiorentino, Italy; [2] Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306, USA

Lorenzo.sorace@unifi.it

Triangular antiferromagnetic spin systems have attracted sustained attention owing to their rich magnetic behavior and relevance to quantum information science, thanks to the significant spin coherence of the transitions involving the two low-lying and almost degenerate ground doublets.[1] In the perspective of investigating spin-electric effects[2] on single-crystals, we report here a combined experimental and theoretical investigation of a Fe_3 spin triangle bridged by a central μ_3-O atom, crystallizing in the acentric *R3* space group (Figure 1). Single crystal data obtained by EPR spectroscopy, flanked by standard and torque magnetometry (CTM), allow us to obtain an unequivocal picture of the lowest lying energy levels of the complex, and evidence clear deviations of the exchange symmetry from the crystallographic C_3 one. First principle calculations demonstrate these deviations are unlikely to arise from intrinsic structural Jahn-Teller distortions. Instead, symmetry-breaking crystal defects or the population of excited vibronic states are found to offer a plausible explanation for effective isosceles exchange and the occurrence of multiple distinct transitions in the EPR spectrum.[3]

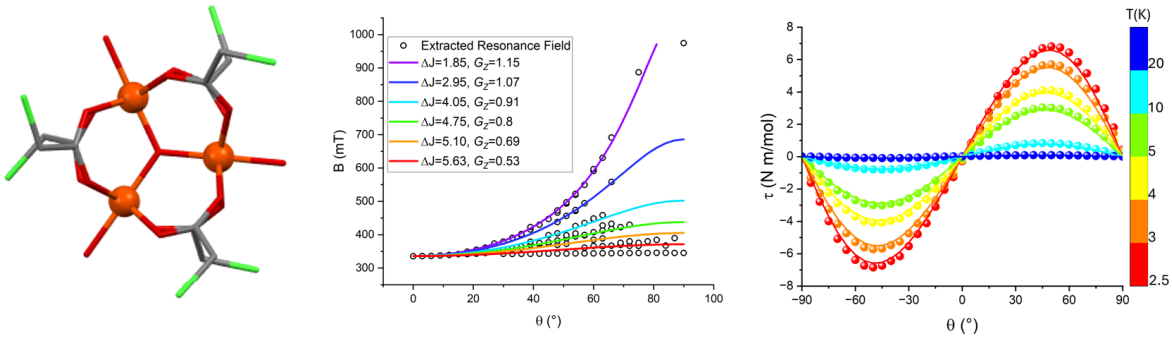

Figure 1: Molecular structure of $[Fe_3O(O_2CCH_2Cl)_6(H_2O)_3]ClO_4 \cdot 9H_2O$, **1**; Experimental and simulated single crystal EPR resonance fields for **1**; Experimental and simulated CTM data for **1**

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HYSDEMON-DEER Correlation Spectroscopy

Maxim Yulikov,[1] Sergei Kuzin,[1,2] Laura Galazzo[1]

[1] ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland; [2] Max Planck Institute for Miltidisciplinary Sciences, Göttingen, Germany

myulikov@ethz.ch

Structural characterization of macromolecular conformational distributions is an emergent important application of pulse EPR. We present a methodology to correlate HYperfine Spectral Diffusion Echo MOdulatioN spectroscopy[1-3] and Double Electron-Electron Resonance spectroscopy[4-6] data for intrinsically disordered proteins. This paves the road to efficiently and quantitatively combining local and long-range structural information in pulse bio-EPR by relating local (within 3 nm) crowding due to peptide chain contacts to the site-to-site distances in the range above 1.8 nm, with the upper limit of several nm, depending on sample deuteration. The presented example of serine-arginine-rich splicing factor 1 (SRSF1) protein in dispersed state offers a simple to interpret proof-of-principle example. A broad variety of applications is anticipated for this new 2D correlation technique, including studies of liquid-liquid phase separation phenomena in biomolecular systems.

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EPR Investigation of Multi-Redox Behavior in Extended TTFs

Michal Zalibera,[1] Viktor Bliksted Roug Pedersen,[2] Jeppe Granhoj,[2] Michal Malček,[1] Israel Fernández,[3] Peter Rapta,[1] and Mogens Brøndsted Nielsen[2]

[1] Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic; [2] University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark; [3] Universidad Complutense de Madrid, 28040 Madrid, Spain

michal.zalibera@stuba.sk

Extended tetrathiafulvalenes (TTFs) with polycyclic aromatic hydrocarbon (PAH) cores undergo stepwise multi-electron oxidation with pronounced changes in electronic structure and spin state.[1,2] EPR spectroscopy combined with UV-Vis-NIR spectroelectrochemistry resolves the charge states and spin characteristics of two PAH-extended TTF families.

Single-electron oxidation generates persistent radical cations with intense NIR absorption and well-resolved EPR spectra. Fluorene- and diindenoanthracene-based systems show PAH-core-dependent spin delocalization confirmed by spin-density calculations.[1] Azulenoazulene-extended TTFs exhibit sequential oxidation tracked by in situ EPR/UV-Vis-NIR spectroelectrochemistry.[2]

Second oxidation produces EPR-silent dications, indicating singlet ground states. In azulenoazulene derivatives, this reflects 22π-aromatic core formation with bond-length equalization supported by X-ray and computational analysis.[2]

These results highlight the power of EPR and spectroelectrochemistry for resolving charge and spin evolution in complex multi-redox organic π-systems.

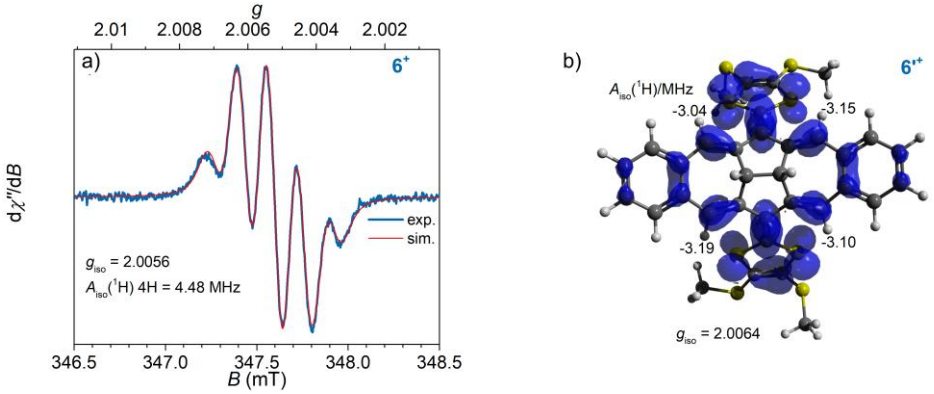

Figure 1: EPR spectrum (a) and spin density (b) of azulenoazulene-extended TTF radical cation.[2]

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

Roberto Zambon,[1] Riccardo Zaramella,[1] Barbara Fresch[1,2]

[1] Università degli Studi di Padova, Dipartimento di Scienze Chimiche, Italy; [2] Università degli Studi di Padova, Padua Quantum Technologies Research Center, Italy

roberto.zambon.2@phd.unipd.it

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 sample inhomogenity and dynamic Jahn-Teller effects, described as incoherent hopping between quasi-degenerate conformations [5]. Finally, we rationalize how a net spin polarization can emerge as non-equilibrium long-living state and how it can be transferred to a radical by dipolar and exchange coupling, considering also the spin-spin relaxation influence.

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Quantum Coherence of Molecular Spin Qubits Hosted in MOFs Studied by EPR Spectroscopy

Dijana Žilić,[1] Lucija Vujević,[1] Fraser MacMillan,[2]

Alexey A. Popov,[3] Bahar Karadeniz,[1] Krunoslav Užarević[1]

[1]Ruđer Bošković Institute, Zagreb, Croatia; [2]Institute of Physics, Zagreb, Croatia; [3]Leibniz IFW, Dresden, Germany

dzilic@irb.hr

The quantum coherence of copper and vanadyl spin qubits hosted in the zirconium porphyrinic metal-organic framework (MOF) PCN-223 was investigated (Figure 1). The properties of the investigated metal qubits were explored using different electron paramagnetic resonance (EPR) techniques such as CW, electron spin-lattice relaxation time (T_1), phase-memory time (T_m), HYSCORE and Rabi oscillation experiments. The results of improving quantum coherence in the investigated molecular spin qubits by mechanochemical spin dilution and fullerene encapsulation in MOF pores will be presented [1, 2].

This work was supported in part by the Croatian Science Foundation under the project numbers HrZZ-IP-2022-10-9292 and HrZZ-IP-2025-02-5083.

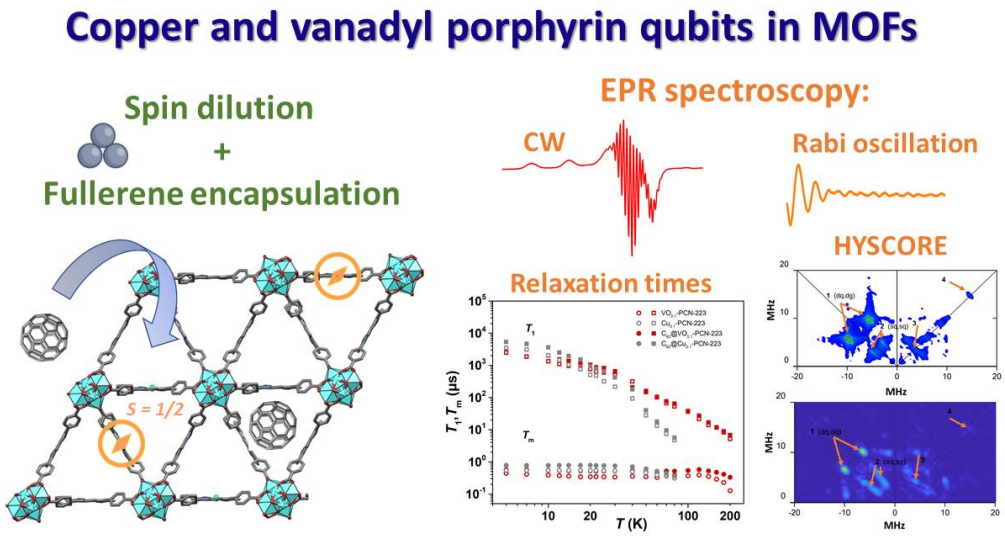

Figure 1: Quantum coherence of molecular spin qubits studied by different EPR techniques.

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Parallel *operando* EPR and contactless conductivity measurements for defects-induced heterogeneous catalysis

Mikhail Agrachev,[1] Katja Raue,[1] Gunnar Jeschke[1]

[1] Department of Chemistry and Applied Biosciences, ETH Zürich, Zürich, Switzerland.

magrachev@ethz.ch

Point defects, such as oxygen vacancies, play a central role in determining the physical and chemical properties of materials. In semiconducting oxides, oxygen vacancies introduce intra-bandgap states and donor levels that strongly modify magnetic, optical, and electrical behavior. They are also produced through Mars-van Krevelen mechanism and act as key active sites in heterogeneous catalysis, including CO_2 hydrogenation and NH_3 oxidation [1–3]. Understanding their evolution under reaction conditions is therefore essential for linking defect chemistry to catalytic performance. As electron-trapping centers (F-centers), they are directly accessible by electron paramagnetic resonance (EPR).

Conductivity in these systems is closely related to defect-induced changes in the band structure of semiconducting supports, particularly through the formation and healing of oxygen vacancies.

Here, we introduce a simple and widely accessible approach that extends continuous-wave (CW) EPR to simultaneous operando measurements of paramagnetic defects and contactless conductivity. By monitoring the microwave diode current of a standard EPR spectrometer, conductivity changes can be detected without hardware modification, enabling direct correlation between EPR-active defect species and charge transport under working conditions.

We demonstrate this method on reducible oxides (In_2O_3, CeO_2), highlighting the role of reducibility, bandgap, and doping. Oxygen vacancy formation increases n-type conductivity and suppresses p-type conductivity, while at high vacancy concentrations, defect band formation leads to exchange-coupled vacancy-bound polarons with distinct EPR signatures. These results establish a direct link between defect formation, electronic structure, and catalytic function.

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Light-activated qubit coupling in a vanadyl porphyrin trimer

Alberto Privitera,[1,2] Alessandro Chiesa,[3] Fabio Santanni,[4] Prem Sahu,[5] Mathias Senge,[4] Matthew Krzyaniak,[2] Ryan Young,[2] Federico Totti,[5] Michael Wasielewski,[2] Stefano Carretta,[3] Roberta Sessoli[5]

[1] Department of Industrial Engineering, University of Florence, Italy; [2] Department of Chemistry, Northwestern University, United States; [3] Department of Mathematical, Physical and Computer Sciences, University of Parma, Italy; [4] School of Chemistry, Trinity College Dublin, Dublin; [5] Department of Chemistry "U. Schiff", University of Florence, Italy

alberto.privitera@unifi.it

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] Recent studies have shown that photoexcitation of a vanadyl porphyrin qubit coupled to a free-base porphyrin chromophore generates a multispin qudit state with spin polarization persisting up to room temperature.[2] A key remaining challenge is the realization of a scalable architecture through the controlled, ultrafast activation of interqubit interactions. Here, we present a molecular system comprising two vanadyl porphyrin qubits ($V^{IV}O$, S=½) bridged by a free-base porphyrin chromophore.[3] The qubits are magnetically independent in the ground state but become coupled upon photoexcitation. Femtosecond transient absorption and time-resolved electron paramagnetic resonance measurements, supported by DFT calculations and spectral simulations, reveal the formation of a spin-quintet state on sub-picosecond timescales with long-lived spin polarization observable up to room temperature. Theoretical modeling provides design principles to establish a proof of concept for light-activated molecular quantum gates. We are currently extending this approach to a broader class of porphyrin-based architectures, with the aim of defining general design rules for exploiting photoinduced processes as a resource for spin polarization and controlled coupling in molecular qubits. This work is supported by the European Research Council (ERC Starting Grant LIGHT-QIS, Project No. 101219747).

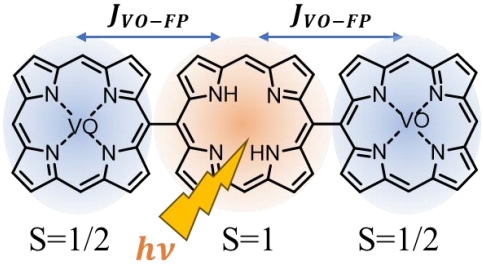

Figure 1: Molecular architecture with two vanadyl porphyrin qubits (VIVO, S=½) bridged by a free-base porphyrin chromophore.

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ESR investigations of the magnetic anisotropy in molecular conductors: Indications of altermagnetism?

Martin Dressel,[1] Zhijie Huang,[1] Mark Kartsovnik[2], Natalia Kushch[3]

[1] 1. Physikalisches Institut, Universität Stuttgart, Germany; [2] Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Germany; [3] Federal Research Center of Problems of Chemcial Physics and Medical Chemistry, Russian Academy of Sciences, Chernogolovka, Russia)

dressel@pi1.physik.uni-stuttgart.de

The two-dimensional molecular conductor κ-$(BETS)_2Mn[N(CN)_2]_3$ has been studied because of the intriguing magnetic coupling of the molecular π-electrons to the Mn^{2+} ions. Utilizing X-band electron spin resonance spectroscopy we have performed comprehensive investigations of the magnetic properties, in particular on the temperature and angular dependences of the spin susceptibility, the *g*-factor, and the linewidth. Due to the π−d coupling, a rearrangement of the π-spins occurs: At low temperatures the *g*-factor shifts enormously with a pronounced in-plane anisotropy that flips as the temperature decreases, the lines broaden significantly, and the spin susceptibility increases upon cooling with a kink at the phase transition. By carefully analyzing the angular dependence of $g(\theta)$ and $\Delta H(\theta)$ we reveal the influence of anisotropic Zeeman interaction in addition to spin-phonon coupling. We conclude the presence of two magnetically distinct BETS chains and discuss the possibility of altermagnetic order.

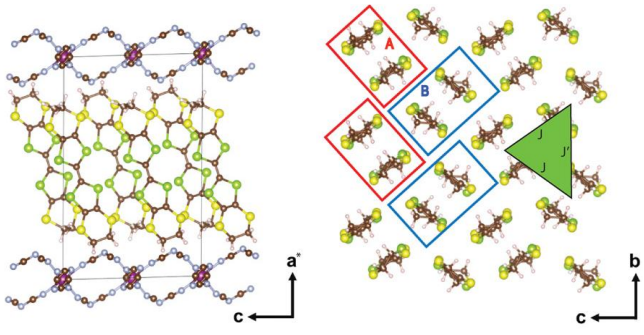

Figure 1: The two-dimensional charge-transfer salt κ-(BETS)2 Mn[N(CN)2]3 forms a layered structure of BETS dimers separated by the bulky $Mn[N(CN)_2]_3^-$ anions, which are formed by Mn^{2+} connected to six neighbors via N ≡ C−N−C ≡ N ligands.
The BETS molecules form distinct dimers A and B are indicated by red and blue squares. They form a triangle as illustrated in green, with the coupling close to frustration $J/J \approx 1$.

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Cryogen-free cryostats and superconducting magnets for EPR and DNP applications

Eugeny Kryukov, Alexander Karabanov, Denis Langlais and Jeremy Good

Cryogenic Ltd, London, UK

eugeny@cryogenic.co.uk

Electron Paramagnetic Resonance (EPR) and Dynamic Nuclear Polarisation (DNP) techniques traditionally rely on superconducting magnets cooled by liquid helium. However, increasing helium costs and limited availability have encouraged the development of cryogen-free superconducting magnets, which operate at temperatures near 4 K without liquid cryogens. Instead, cooling is achieved using a closed-cycle refrigeration system consisting of a cold head and a helium gas compressor.

Cryogen-free cryostats and superconductive magnets offer several advantages for EPR applications. Their compact design eliminates the need for large liquid helium and nitrogen reservoirs, reducing both operational complexity and laboratory space requirements. They also improve safety by avoiding risks associated with helium boil-off and pressure build-up during a magnet quench as well as the risk of suffocation.

An important feature of the cryogen-free systems is the integrated Variable Temperature Insert (iVTI), which enables precise sample temperature control from approximately 1.3 K to 300 K. This is particularly valuable in EPR, where temperature strongly influences spin relaxation and molecular dynamics. In addition, cryogen-free magnets allow possibility to run experiments at different magnetic fields, typically from about 500 Gauss up to the magnet's maximum field, without any extra cost [1].

Cryogen-free technology is increasingly used in EPR, solid state NMR, MRI and DNP. For EPR specifically, it provides greater accessibility to low-temperature and variable-field experiments while reducing dependence on liquid helium infrastructure. The field stability in cryogen-free magnets achieved requirements for all methods listed above. With some extra correction such magnet can be used also in liquid state NMR [2].

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Expanding the Reach of EPR: Distance Measurements and Applications in Quantum Information Science

Maximilian Mayländer[1]

[1] Bruker BioSpin GmbH & Co KG, Rudolf-Plank-Str. 23, 76275 Ettlingen, Germany

m.maylaender@bruker.com

Microwave pulse shaping has emerged as a powerful approach for expanding the capabilities of modern EPR spectroscopy. In structural biology, shaped microwave pulses significantly improve the performance of pulsed EPR techniques such as Double Electron Electron Resonance (DEER/PELDOR)[1] and Single Frequency Technique for Refocusing Dipolar Couplings (SIFTER)[2] by enabling more uniform and broadband excitation.[3–6] At the same time, emerging applications in quantum information science demand not only broadband operation but also high-fidelity control of spin qubits, including precise state preparation, manipulation, and readout. Addressing this broad range of requirements within a single experimental platform calls for an architecture that is both flexible and highly controllable.

To meet these demands, we developed microwave resonators that provide high B_1 uniformity and tunable B_1 bandwidth based on a loop-gap architecture, enabling accurate control over excitation conditions. We further integrated an arbitrary waveform generator using an intermediate-frequency scheme, which allows efficient manipulation of pulse bandwidth, shape, and spectral position across the EPR range. This combination supports high-fidelity spin control suitable for both structural biology and quantum-technology applications.

Together, these developments establish versatile EPR platforms capable of delivering uniform broadband excitation, precise pulse shaping, and high-fidelity spin manipulation, addressing the individual needs from structural biology to spin-based quantum technologies.

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New functionalities in multiharmonic analysis

Czechowski T[1], Baranowski M[1,2], Szczepanik P[1], Jurga P[1], Malinowski P[1]

[1]Novilet, Poznan, Poland; [2]Faculty of Physics and Astronomy, Adam Mickiewicz University in Poznan, Poland

t.czechowski@novilet.eu

Multiharmonic analysis has been developed for years [1–5] and enables, among other things, the reconstruction of the unmodulated shape of CW EPR spectra regardless of the modulation amplitude used. Ultimately, the quality of the obtained signals is influenced by experimental parameters, hardware parameters, and the analysis algorithms used. Properly performed multiharmonic analysis requires consideration of a number of factors, in particular: the impact of the detection bandwidth on the recorded harmonics and the passage effect in the recorded data.

The solutions used in the new algorithm allow for the correction of these effects and the acquisition of spectra unaffected by these factors. Firstly, this results in signal reconstruction with the highest possible efficiency, even if the signal's bandwidth was wider than the detection bandwidth. Secondly, it is possible to perform multiharmonic analysis for radicals for which the passage effect known from the rapid scan technique is observed on the harmonics, which is corrected during the analysis. Additionally, the procedures used in the multiharmonic analysis algorithm to optimize the noise parameters of the spectrum provide an above-average increase in sensitivity. The use of multiharmonic analysis results in a multiple increase in the signal-to-noise ratio of the spectra, which, depending on the experimental conditions, can reach up to two orders of magnitude.

It should be emphasized that the development and practical implementation of multiharmonic analysis has been significantly advanced thanks to the work of Novilet, whose technological solutions and innovative algorithms played a key role in refining this technique. Multiharmonic analysis can be performed on Novilet ERI DUO imagers or as an add-on to existing or new Bruker EPR spectrometers.

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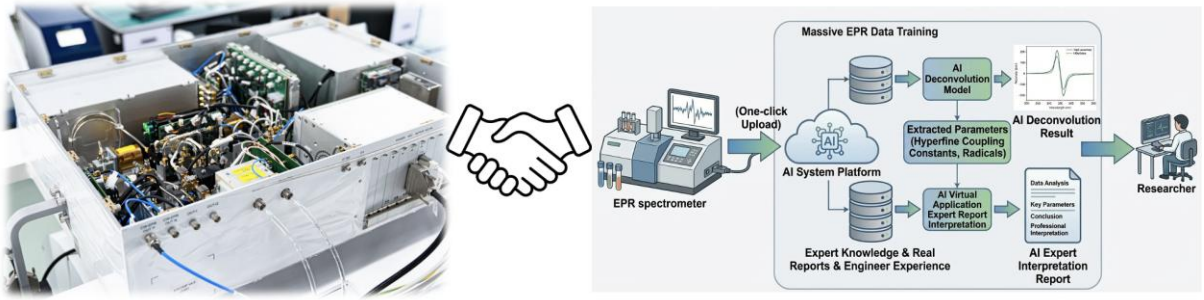
Next-Generation EPR: Combining High-Performance Q Band Instrumentation with Artificial Intelligence Enhanced Spectral Processing

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

CIQTEK Co., Ltd., No. 1969, Kongquetai Road, HeFei High Tech Zone, AnHui, China

Keywords: Q Band EPR, AI Spectral processing, Automatic Report Generation, Solid-State Power Amplifier



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

Our Q-band pulsed EPR system achieves less than 10 ns π/2 pulse wide-bandwidth excitation using a Solid-State Power Amplifier, offering superior longevity and reduced maintenance over conventional technology. This architecture maximizes sensitivity and spectral resolution, deciphering complex metal hyperfine couplings and extracting dipolar information for high-resolution DEER distance mapping.

Complementing the hardware is a three-layer AI EPR model that streamlines the workflow from raw data to publication. Trained on over 100,000 real and simulated datasets — achieving 99.9% precision for simulations and 92% for real-world samples — the model automates spectral fitting, component characterization, and experimental report generation. It further offers predictive guidance, suggesting follow-up experiments to validate findings.

This integrated approach lowers the entry barrier for researchers in chemistry, biology, and materials science, driving EPR toward a more impactful technology.

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CONTRIBUTING TALKS

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From Single Crystal to Powder: Magneto-Structural Correlation in Cu(salen) complex revealed by HFEPR

Arenas D.[1*], Lima L.[1], Santiago P.[1], Kotásková L.[1], Sartoris, R.P.[2], Santana V.T.[1]

[1] Central European Institute of Technology, Brno University of Technology, Brno, 61200, Czech Republic;
[2] Departamento de Física, Facultad de Bioquímica y Ciencias Biológicas, Universidad Nacional del Litoral (UNL), 3000 Santa Fe, Argentina

arenas@vutbr.cz

Low-dimensional coordination compounds with bridging ligands are an important research topic due to their relevance in molecular magnetism and their potential to serve as single-molecule magnets, single-chain magnets, and metal-organic magnets[1]. In recent years, our group has studied the magneto-structural properties of dimeric and monomeric Cu coordination compounds using high-frequency electron paramagnetic resonance (HFEPR)[2,3]. The physical properties of these compounds are characterized by isotropic exchange and anisotropic spin-spin interactions[4]. In this context, we investigate the compound [Cu(salen)] (salen = (*N*,*N'*-ethylene-bis(salicylidenimine)), which has magnetically different dinuclear units correlated by a 180° rotation about the *b* axis within the unit cell, forming 2D layers. HFEPR measurements were performed at 95 GHz and above 300 GHz, applying a magnetic field ($\mathbf{B_0}$) up to 16 T at room temperature in both powder and oriented single crystal samples. Powder EPR spectra suggest rhombic symmetry at 95 GHz, but additional lines observed at higher frequencies cannot be explained in the same way. Single crystal spectra at 329 GHz revealed that the system's dynamics consist of two phases driven by the weak intermolecular exchange *J'*, where the dinuclear units display merged or split EPR peaks according to the orientation of $\mathbf{B_0}$. Finally, we analyzed the data to determine the crystal and molecular g-tensors and calculate $|J'| \sim 0.2$ cm^{-1}.

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Optimising Rapid Scan EPR for the kinetic study of light-induced processes

Saverio B. Canu[1], Adam Brookfield[1], Murali Shanmugam[1], Alexander Golovanov[1], David Collision[1], Alice M. Bowen[1].

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

saverio.canu@postgrad.manchester.ac.uk

Rapid Scan Electron Paramagnetic Resonance (RS-EPR) is an emerging continuous-wave (CW) technique that offers a significantly enhanced signal-to-noise ratio (SNR) and superior temporal resolution compared to conventional field-modulated CW-EPR[1]. A primary advantage of RS-EPR is its high acquisition speed making it exceptionally well-suited for the kinetic study of light-induced processes. Here we present our work towards the development of novel methodologies for time-resolved RS-EPR with in-situ illumination, utilizing the recently released commercial Bruker Rapid Scan (RS) accessory[2]. We have successfully developed a time-resolved setup with a resolution of 35 ms and validated this by observing the spin-trapping of photo-generated hydroxyl radicals from H_2O_2 using DMPO; in-situ illumination was achieved via the EPR-torch method[3]. Subsequently we have exploited the full temporal resolution of the RS instrument (up to 10 µs) for optically initiated experiments, by integrating Xepr API scripting with an external pulse generator. This overcomes the hardware constraints that limit the number of acquirable RS slices. Additionally, a known limitation of RS-EPR is its restricted scan width, which complicates the characterization of broad spectral features. To circumvent this, we have implemented a "stitching" protocol to combine multiple RS traces. Using 100G wide RS slices, a 4000G wide spectrum was successfully reconstructed, with background artifacts efficiently removed via Fourier filtering.

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IMPLEMENTING PULSE EPR WITH SHAPED PULSES FOR ROUTINE STRUCTURAL STUDIES

Aisika Chakraborty, Katrin Ackermann, Bela E. Bode

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

ac523@st-andrews.ac.uk

Bio-macromolecular ensembles like proteins and nucleic acids underpin all functions of life. Studying the structure and interactions of these molecules helps understanding biomolecular mechanisms related to health and disease. Pulse Dipolar Electron Paramagnetic Resonance (EPR) Spectroscopic (PDS) techniques along with site-directed spin-labelling have been popularized for measuring distances in the nanometre-range which contributes to confirming or rejecting structural models (such as those generated by Alphafold2/3) and conforming regions of disorder. Thus, providing deeper insights about dynamic processes, conformational equilibria and ensemble distributions in solution. The most broadly applied PDS experiment in this context is the Pulse Electron-Electron Double Resonance (PELDOR aka DEER) technique[1] with a pulse sequence, that recovers the magnetic dipole-dipole coupling between two or more paramagnetic centres, which contains information about the distance distribution between them. However, the most challenging applications are still limited by sensitivity and distance resolution. The development of the 5-pulse PELDOR[2] has extended the accessible dipolar evolution time and thus increased the measurable distance range compared to the most used 4-pulse experiment. Despite these advantages, 5-pulse PELDOR is more prone to pulse imperfections, leading to the formation of signals from unwanted dipolar pathways[3]. These artefacts can distort the dipolar signal and, if not properly treated, may result in erroneous distance analysis. A detailed characterisation and separation of desired and undesired pathways is therefore essential, particularly when studying systems with broad or multimodal distance distributions.

In this project, practice implementation of 5-pulse PELDOR resulted in an approximately threefold increased signal to noise ratio (SNR) relative to 4-pulse PELDOR or alternatively enabled an extension of the dipolar evolution time window while maintaining comparable sensitivity. The project further aims to systematically compare 4-pulse and 5-pulse PELDOR for systems exhibiting complex and overlapping distance distributions. Emphasis is placed on evaluating the impact of pulse imperfections, pathway selection, and refocusing efficiency on the reliability of extracted distance distributions. By establishing criteria for reliable pathway discrimination and studying the trade-offs between sensitivity, time window, and artefact suppression, this work seeks to define the conditions under which 5-pulse PELDOR can be robustly applied for routine structural studies of biomacromolecules with complex conformational ensembles.

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High field EPR and ^{13}C DNP of NV centers in Diamond

A. Hecht, E.Laster, A. Fialkov, N. Manukovsky, I. Kaminker

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

ayalahecht@mail.tau.ac.il

Nitrogen-Vacancy (NV) centers are paramagnetic defects in diamonds that consist of a Nitrogen atom substituting for a Carbon atom, and a negatively charged vacancy adjacent to the substitution, forming an **S=1** paramagnetic system. NV centers emerged as promising candidates for multiple applications, such as quantum computing, quantum sensing, and imaging of biological processes [1]. The uniqueness of NV centers stems from the **coupling between their spin and optical properties** combined with long coherence times at room temperature. For example, illuminating the diamond sample with **green light preferentially populates the m_s = 0 state**, resulting in a substantial increase in electron spin polarization and, as a result, increased EPR signal intensity (see fig.1) [2]. The extent of polarization depends on the NV center orientation with relation to B_0.

Dynamic Nuclear Polarization (DNP) is a signal enhancement technique in NMR spectroscopy that is based on polarization transfer from the electron spins to nuclear spins. Typically, the Boltzmann electron spin polarization sets the theoretical limit on maximal achievable nuclear polarization. Increasing electron spin polarization beyond the Boltzmann limit helps alleviate this limitation and to **transfer more polarization to the nuclei** surrounding the electrons via established DNP mechanisms [3].

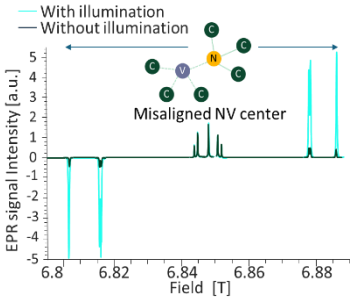

Fig.1 - Field sweep spectrum of diamond at 191.9 GHz

An improvement in resolution forces contemporary NMR spectroscopy to high magnetic fields hence the DNP experiments have to be performed at high fields as well. The NV centers are usually studied at low fields (up to 0.3 T). In this work we present pulsed EPR and DNP results on optically polarized NV centers at 7 and 14 T. Seeking to understand the dependence of ^{13}C DNP efficiency on electron polarization, we examined the dependence of DNP enhancement on the NV center orientation with relation to B_0. We discovered an unexpected asymmetric pattern in solid-effect efficiency in ^{13}C DNP experiments performed with NV centers tilted relative to the magnetic field.

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Direct Detection of MAS-induced Polarization Exchange in P1 Centers by High-Field MAS-EPR

Sudipta Khamrui,[1] Orit Nir-Arad,[1] Frederic Mentink-Vigier,[2] Alexander B. Fialkov,[1] Nurit Manukovsky,[1] Ilia Kaminker[1]

[1] School of Chemistry, Faculty of Exact Sciences, Tel-Aviv University, Israel; [2] National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA.

sudipta20102@tauex.tau.ac.il

Dynamic Nuclear Polarization (DNP) enhances the sensitivity of Nuclear Magnetic Resonance by transferring polarization from an unpaired electron spin to neighbouring nuclear spins. The development and optimization of DNP require a thorough understanding of electron spin dynamics, obtainable only through pulsed-EPR. Since DNP performance is condition-dependent, typical low-field static EPR experiments are of limited relevance for contemporary high-field Magic Angle Spinning (MAS) DNP, necessitating high-field pulsed MAS-EPR instrumentation and methodology. Recently, we reported the first high-field MAS-EPR experiments with up to 3 kHz spinning rate [1], enabling observation of electron spin dynamics on a few microsecond timescales. However, electron-nuclear polarization transfer in DNP typically occurs over a longer period.

This work presents rotor-synchronized 3-pulse stimulated echo detected MAS-EPR with up to a 37 kHz spinning rate at 6.9 T, allowing to observe electron spin dynamics on the hundreds of µs timescale (Fig 1b). We observe that the echo decay rate increases with MAS rate (Fig 1c), attributed to decreased efficiency of spinning-induced polarization exchange between different electron spins. MAS enables e^--e^- polarization exchange because the resonance frequencies of different spin packets transiently overlap due to the frequency shift upon sample reorientation under MAS. Crucial for DNP, the efficiency of this polarization exchange depends on the EPR line anisotropy, MAS rate, and the strength of the e^--e^- dipolar interaction. Here, for the first time, we demonstrate that the efficiency of polarization exchange can be directly measured by MAS-EPR. This work constitutes a step toward the rational design of DNP experiments.

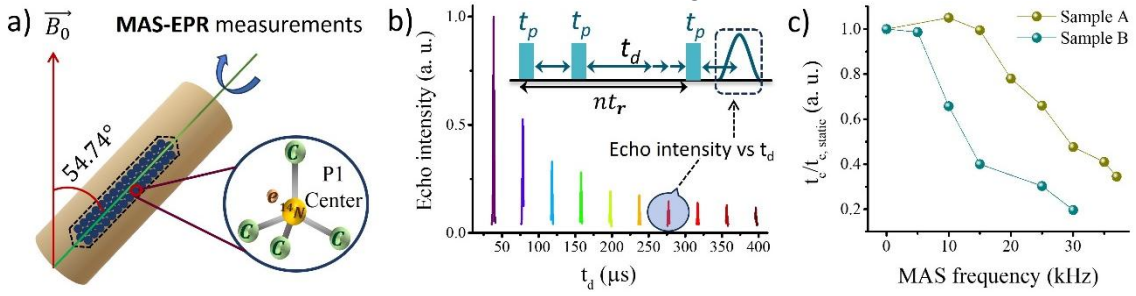

Figure 1: (a) MAS-EPR measurements setup. b) 3p-echo intensity vs delay time at 25 kHz spinning. c) 3p-echo decay rate vs MAS rate for two different diamonds, normalised with respect to static time constant.

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Investigating Surfactant–Alginate Interactions: Surface Tension and Nanostructure Modulation for Biomedical Applications

Khuram shehzad Khan,[1] Carlo Carandente Coscia,[2] Matilde Tancredi,[2] Gerardino D'Errico,[2] Luigi Paduano,[2]

[1] Department of Molecular Sciences for Earth and Space (MOSES), Scuola Superiore Meridionale, Via Mezzocannone, 4 - 80138 (NA), Italy; [2] Department of Chemical Sciences, University of Naples Federico II, Complesso Universitario Monte Sant'Angelo, Via Cinthia 4, 80126 Naples, Italy

ks.khan@ssmeridionale.it

My research focuses on investigating surfactant–alginate interactions as a foundation for the design of nanostructured bio-based hydrogels, with an emphasis on natural polysaccharides as key biopolymeric matrices. The rational design of biopolymer-based hydrogels requires a deep molecular-level understanding of polymer-surfactant interactions. This study investigates the interaction of sodium alginate with single (CTAB, SDS, Tween 80) and mixed surfactant systems (C_{10}En/CTAB) using surface tension, Dynamic Light Scattering (DLS), and Electron Paramagnetic Resonance (EPR) spectroscopy. Using 5-doxylstearic acid (5-DS) as a spin probe, EPR spectra revealed a distinct two-phase transition as a function of surfactant concentration. In the pre-micellar regime (<0.5 mmol kg^{-1}}, a sharp, steep increase in the rotational correlation time (τ_c) indicates the early formation of rigid polymer-surfactant complexes that restrict probe mobility. Beyond the critical micelle concentration, spectral simulation unveiled a complex, multi-component dynamic environment. The EPR spectra were successfully resolved into two distinct components: a slow-diffusing component ($\tau_c \cong$ 0.95nc) corresponding to probes immobilized within alginate-bound mixed aggregates, and a faster-diffusing component ($\tau_c \cong$ 0.54 ns) viscosity and micro-environmental crowding provide a structural roadmap for fabricating tailored nanostructured hydrogels for optoelectronic and biosensing applications.

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Bridging Molecular Electron Spin Qubits via Photoactive Arenes to Enable Switching of Coupling Interactions

Lubomir Loci,[1] O. P. Churchill,[1] O. L. Kanibolotskyy,[2] D. J. Heyes,[1] E. J. L. McInnes,[1] P. Skabara,[2] A. M. Bowen,[1] R. E. P. Winpenny[1]

[1] Department of Chemistry and National Research Facility for EPR, University of Manchester, Oxford Road, Manchester, M13 9PL, UK; [2] School of Chemistry, University of Glasgow, Joseph Black Building, University Place, Glasgow, G12 8QQ, UK.

lubomir.loci@manchester.ac.uk

Molecular paramagnetic systems could be used to implement Quantum Information Processing (QIP) algorithms, since electron spins can be precisely controlled by magnetic resonance techniques. However, to perform non-trivial calculations, operations involving a single qubit and those involving two coupled qubits (known as one- and two-qubit gates) are both required.

Here, we investigate whether an arene bound to two {Cr_7Ni} rings[1] (Figure 1) can act as a light-induced qubit switch. Time-resolved EPR (TREPR) and Transient Absorption (TA) measurements show the isolated arene can be photoexcited to a triplet state with good quantum yield. However, on analogous photoexcitation of the arene bound to {Cr_7Ni}, the spin polarisation pattern of the arene triplet signal is altered in the TREPR. Additionally, signal belonging to the polarised ground state of the two {Cr_7Ni} rings is observed. These results may be indicative of arene-to-ring energy transfer and considerable inter-spin coupling, as observed recently for a porphyrin-ring complex.[2]

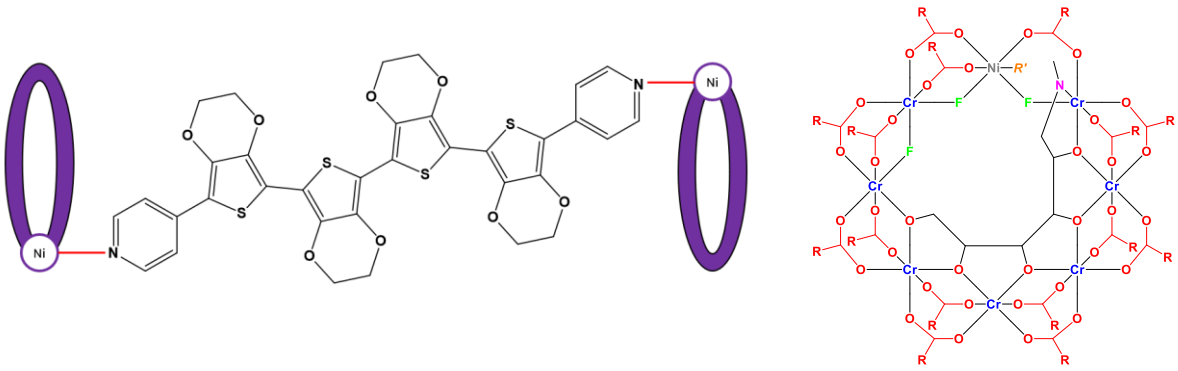

Figure 1: (left) Visualisation of the ring-arene-ring system. (right) Skeletal formula of {Cr_7Ni} rings.

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High-Frequency Electron Spin Resonance Spectroscopy of Layered Magnets

Shibnath Mandal,[1] Oleksii Laguta,[2] Petr Neugebauer[2], Subhadeep Datta[1]

[1]School of Physical Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata - 700032, India; [2]Central European Institute of Technology, Brno University of Technology, Purky\v nova 656/123, 61200 Brno, Czech Republic

shibnathmandal7663@gmail.com

Magnetism in two-dimensional (2D) materials is governed by the interplay between magnetic anisotropy and interlayer exchange. While an ideal isotropic 2D Heisenberg system cannot sustain long-range order at finite temperature due to thermal fluctuations, anisotropy opens a spin-wave gap that stabilizes magnetic order. In real materials, magnetic anisotropy together with weak interlayer exchange stabilizes long-range order by introducing quasi-three-dimensional behavior. Notably, the low values of anisotropy and interlayer exchange (in order of μeV) can be challenging to detect using conventional techniques such as neutron scattering. Here, we use high-frequency ESR (90 to 1100 GHz) to probe the anisotropy field and interlayer exchange coupling in a 2D magnet. A resonance mode corresponding to the zero-field resonance condition is identified as the ferromagnetic resonance (FMR) mode, while an additional resonance mode corresponds to an interlayer exchange–driven excitation. This zero-field FMR mode represents the uniform, in-phase precession of spins within each layer. In contrast, the additional resonance mode arises from an out-of-phase precession between adjacent layers, reflecting the presence of weak interlayer exchange coupling that lifts the degeneracy and leads to mode splitting. This zero-field resonance frequency information about the magnetic anisotropy of the system, while the field separation between the two resonance modes gives insight into the strength of the interlayer exchange coupling.

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When is Five better than Four? Applications of 5P DEER for Distance Measurements in Challenging Biomolecular Systems

Alysia Mandato,[1] Jorden Seru,[1] Hugo Karas,[1,2] Svetlana Kucher,[1] Enrica Bordignon[1]

[1] Department of Physical Chemistry, School of Chemistry and Biochemistry, Faculty of Science, University of Geneva, Geneva, Switzerland

[2] Department of Chemistry and Applied Biosciences, ETH Zürich, Zürich, Switzerland

Alysia.Mandato@unige.ch

Five-pulse double electron–electron resonance (5P DEER) spectroscopy offers the potential for extended dipolar evolution times and improved sensitivity compared with conventional four-pulse DEER (4P DEER).[1] An important practical question, however, is when the additional experimental complexity translates into improved structural information. 5P DEER remains less widely used due to increased complexity of the experiment and analysis, which requires the treatment of additional dipolar pathways. Recent developments in DeerLab[2] and DeerAnalysis2026 have simplified the analysis of 5P DEER data, providing an opportunity to more systematically evaluate the advantages and limitations of the technique across a range of experimental systems.

In this work, we compare 4P and 5P DEER measurements for samples across several common distance measurement scenarios. These include narrow and broad unimodal distance distributions in model biradicals and proteins, bimodal distributions from mixed or conformationally heterogenous systems, and membrane-associated proteins exhibiting non-3D backgrounds. The examples were selected to represent levels of experimental complexity and situations where longer dipolar evolution times are expected to provide additional structural information.

The resulting comparisons are used to assess when 5P DEER provides measurable improvements over conventional 4P DEER and when the simpler experiment is sufficient. Additionally, we highlight practical analysis methods using DeerLab, including treatment of multiple dipolar pathways and background modeling. We are working to extend these comparisons to increasingly complex environments, including mitochondrial and cellular measurements and alternative spin systems such as Gd(III) and Cu(II). Our goal is to provide practical guidance to the biophysical community for the choice and analysis of 5P DEER experiments.

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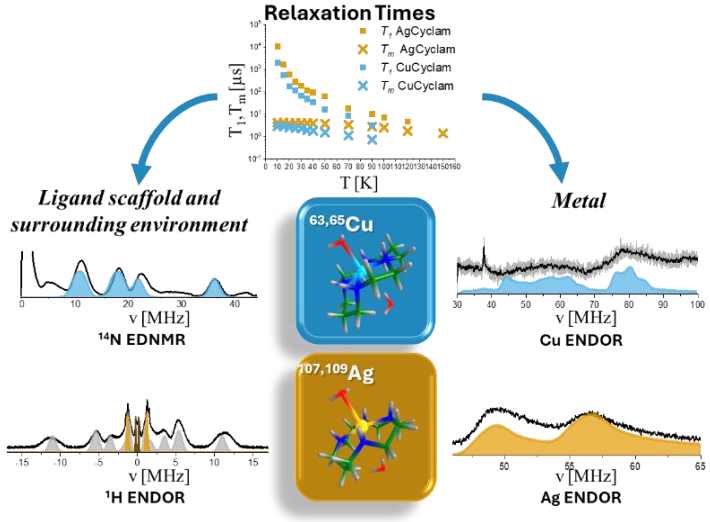
Periodic trends in electronic structure and spin relaxation across Cu(II) and Ag(II) complexes.

Maria Chiara Pagliero,[1] Paolo Cleto Bruzzese,[1] Marco Ricci,[2] Mauro Botta,[2] Fabio Carniato,[2] Enrico Salvadori,[1] Mario Chiesa.[1]

[1] Università di Torino, Dipartimento di Chimica, Torino, Italia
[2] Università del Piemonte Orientale, Dipartimento di Scienze e Innovazione Tecnologica, Alessandria, Italia

mariachiara.pagliero@unito.it

Designing paramagnetic transition metal complexes for spin-based technologies requires a detailed understanding of the geometric and electronic factors governing electron spin relaxation.[1] Among these, electronic structure, spin–orbit coupling, ligand field effects, and spin delocalization play central roles.[2] Periodic trends are expected to influence all these parameters. Here, we investigate the differences in relaxation properties and electronic structures of isoelectronic Cu(II) and Ag(II) complexes, selected as a model 3d/4d pair, featuring an identical macrocyclic ligand scaffold and coordination environment. By combining hyperfine spectroscopies with density functional theory (DFT) calculations, we obtain a comprehensive picture of spin density distribution, metal–ligand covalency, and chemical bonding.



In parallel, measurements of electron spin relaxation times (T_1 and T_m) reveal slower relaxation in the Ag(II) complex compared to its Cu(II) analogue, a trend that is not trivially anticipated from spin–orbit considerations alone and reflects the interplay of covalency and magnetic anisotropy. The combined experimental and computational analysis highlights how periodic trends modulate spin distribution and relaxation pathways.

These findings provide valuable insights for the rational design of transition metal complexes with tailored spin delocalization and relaxation properties for quantum and spintronic applications.

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Multiphoton Double Electron Electron Resonance

I.Petkov,[1] S. Lockyer,[1] A. Brookfield,[1] L. Loci,[1] M. Tasfina,[1] A. Golovanov,[1] E. J. L. McInnes,[1] R. E. P. Winpenny,[1] A. M. Bowen[1]

[1] Department of Chemistry, University of Manchester, Oxford Road M13 9PL Manchester, United Kingdom

ivan.petkov@manchester.ac.uk

Transitions between spin states can be realised using multiple photons, passing through virtual states and described by Floquet theory[1]. With both microwave (mw) and radiofrequency (rf) sources, resonances can be observed at frequencies of ω_{mw}, $\omega_{mw} \pm \omega_{rf}$, $\omega_{mw} \pm 2\omega_{rf}$ etc. The transition probabilities for the various resonances can be manipulated with the choice of rf power and rf frequency used, and the ω_{mw} resonance can be made to disappear entirely, in a 'π-photon-induced-transparency' condition [2],[3]. This project demonstrates the use of the 'π-photon-induced-transparency' condition in a multiphoton version of the Double Electron Electron Resonance (DEER) experiment. Here, the pulse with simultaneous mw and rf (Figure 1) excites only resonances at frequencies which are distinct from those excited by the other pulses. This satisfies the frequency-difference requirement of DEER using just one mw frequency, which has the potential to bypass the limitations of pulse power and bandwidth that come from over-coupling the EPR resonator.

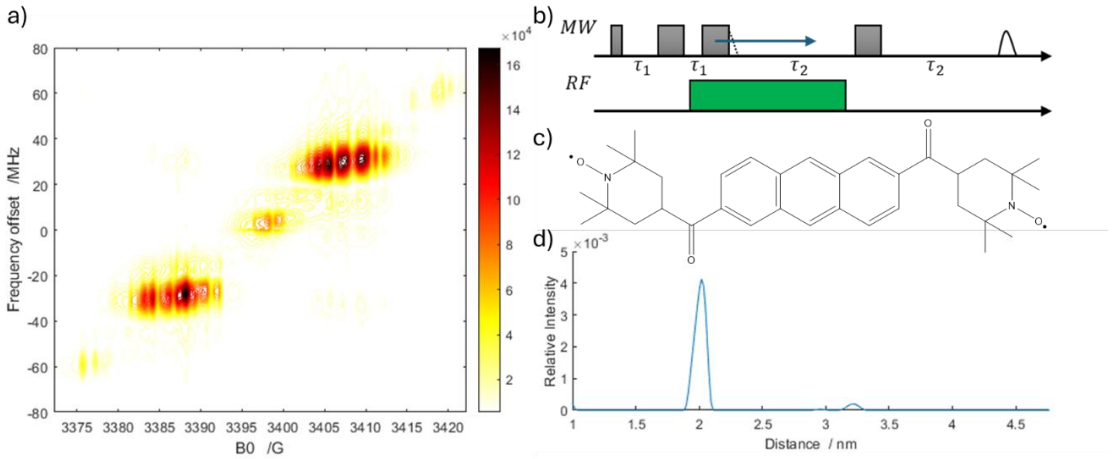

Figure 1: a) Multiphoton transitions observed for a Hahn echo with simultaneous mw and rf pulses on coal. b) Multiphoton DEER pulse sequence. c) A nitroxide biradical, for which d) shows the distance distribution obtained following a multiphoton DEER experiment.

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Modelling Purcell-Limited Spin Relaxation in Inhomogeneous Microresonator Magnetic Fields

Aistė Peštenytė,[1] Gediminas Usevičius,[1] Jūras Banys,[1] John J.L. Morton,[2,3] Mantas Šimėnas[1]

[1]Faculty of Physics, Vilnius University, Saulėtekio al. 3, LT-10257, Vilnius, Lithuania; [2]London Centre for Nanotechnology, University College London, London WC1H 0AH, UK; [3]Dept. of Electronic & Electrical Engineering, University College London, London WC1E 7JE, UK

aiste.pestenyte@ff.stud.vu.lt

With the rapid development of quantum technologies, there is an increasing demand for reliable and well-controlled physical systems. Due to their potentially long coherence times, electron spins are considered promising candidates in this context [1]. As a result, electron spin resonance (ESR) has become an important tool for studying spin systems, as it allows direct probing of spin states. In many ESR experiments of spin qubits, measurements are performed at millikelvin temperatures in order to reduce thermal noise, increase spin polarization, and preserve long coherence times. At such low temperature, the spin-lattice relaxation time (T_1) increases significantly, making experiments impractical and technically challenging. To address these challenges, superconducting microwave resonators with high Q-factors are often used. Such resonators amplify the field experienced by the spins, boosting the spin-resonator coupling. An increase in coupling strength leads to the Purcell relaxation effect, which significantly accelerates spin relaxation enabling ESR experiments [2].

In this work, we solve the Bloch equations for various pulse sequences where spin relaxation is limited by the Purcell effect only in the presence of a straight inductor of a superconducting microwave resonator. This framework allows us to study how spatial variations in the spin-resonator coupling and the driving microwave field affect spin relaxation dynamics. The model provides insight into Purcell-limited relaxation in microresonator-based ESR experiments and serves as a basis for further investigations.

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Analysis of paramagnetic probe OX071 pharmacokinetics in mice between different administration methods.

Radzikowska N.,[1] Dziurman G.,[1,2] Krzykawska-Serda M.[1], Elas M.[1]

[1] Department of Biophysics and Cancer Biology, Jagiellonian University, Krakow, Poland; [2] Doctoral School of Exact and Natural Sciences, Jagiellonian University, Krakow, Poland;

natalia.radzikowska@student.uj.edu.pl

EPR pulse imaging relies on the trityl family oximetric spin probes due to their high sensitivity to oxygen and lack of toxicity. In this study, we aimed to compare the pO_2 images and the pharmacokinetics of an oxygen-sensitive probe OX071 between two groups of mice differing in administration routes of the spin probe: intraperitoneal (IP) or intravenous (IV). The analysis focuses on changes in distributions of the amplitude of the spin probe signal and pO_2. We have analysed voxel behaviour between the beginning and end of the imaging process. Voxels were divided into amplitude-based quantile groups to evaluate shifts in their average positions over time. The results indicate that the probe kinetics differ between IP and IV administration, with more pronounced voxel shifts observed in the IV group, especially along the amplitude axis. In both groups, changes in amplitude ranges were observed during the imaging process, suggesting dynamic redistribution of the probe signal over time. Statistical analyses were performed to compare voxel shifts between groups and to investigate potential relationships with physiological parameters. These findings may help improve the selection of the optimal time window for oxygen imaging in living animals.

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Distance measurements with ^{19}F time domain ENDOR spectroscopy on RNA model systems

M. L. Rämisch[1,2*], L. Sielaff [1,2], Sergei Kuzin[2], F. Seitz [3], A. Meyer[1,2], C. Höbartner [3], M. Bennati [1,2]

[1] Research Group EPR Spectroscopy, Max Planck Institute for Multidisciplinary Sciences, Am Faßberg 11, 37077 Göttingen, Germany; [2] Institute of Physical Chemistry, Georg-August-Universität Göttingen, Tammannstraße 6, 37077 Göttingen, Germany; [3] Institute of Organic Chemistry, University of Würzburg, Am Hubland, 79074 Würzburg, Germany

maya.raemisch@mpinat.mpg.de

Pulsed Dipolar Hyperfine Spectroscopy (PDHS) is a newly developed ^{19}F-ENDOR technique that detects nuclear hyperfine modulations directly. By separating electron-nuclear dipolar couplings from other line-broadening interactions, PDHS achieves significantly improved spectral resolution compared to frequency-domain ENDOR, pushing the current limits of ENDOR-based distance measurements in biomolecular systems.[1] Here, we applied PDHS to four RNA duplexes (Fig. 1A), site-specifically labelled with TEMPO and ^{19}F, with defined inter-spin distances of 12-21 Å.[2] The intrinsic flexibility of both RNA and the TEMPO spin label, combined with a ^{1}H background arising from overlapping ^{1}H and ^{19}F resonances at Q-band frequencies (34 GHz), poses significant challenges for the analysis. We present an approach that enables reliable PDHS measurements on fully protonated samples without the need for RNA deuteration or specialized hardware. Validated through complementary measurements, this approach yields distance distributions (Fig. 1B) that provide insights into the structural flexibility and dynamics of RNA, supported by computational modelling. These results demonstrate the applicability of PDHS to biological systems and pave the way for future ^{19}F time-domain ENDOR studies on more complex biosystems. To extend the accessible distance range, we explore CF_3 groups as ^{19}F spin labels, offering substantially higher sensitivity and enabling measurements beyond current limits.

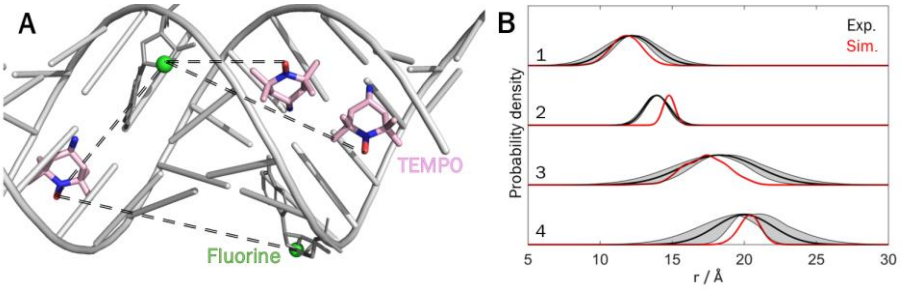

Figure 1: A: RNA model system demonstrating the four different distances. B: Distance distributions obtained by time domain pulsed dipolar hyperfine spectroscopy.

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Defect Chemistry and Interfacial Transport in Titanium Oxide-Based Anodes for Solid-State Lithium Batteries

Shoaib Nazir,[1]

[1]College of Materials Science and Engineering, Shenzhen University, Shenzhen 518060, China

comsian.shoaib@gmail.com

Titanium oxide-based anodes, including TiO_2 polymorphs, $Li_4Ti_5O_{12}$ (LTO), and $TiNb_2O_7$ (TNO), are promising candidates for solid-state lithium batteries because of their structural stability, safety, and low-strain lithiation behavior [1]. However, poor electronic conductivity and interfacial charge-transfer resistance limit their practical performance. This work highlights recent advances in defect-regulated titanium oxide systems, focusing on heteroatom substitution, oxygen-vacancy engineering, and interfacial stabilization strategies for improving Li^+ transport kinetics and electrochemical stability [2]. The relationship between defect chemistry, local electronic structure, and solid-solid interfacial transport is discussed to provide design principles for safe, fast-charging, and durable solid-state lithium batteries (Figure 1).

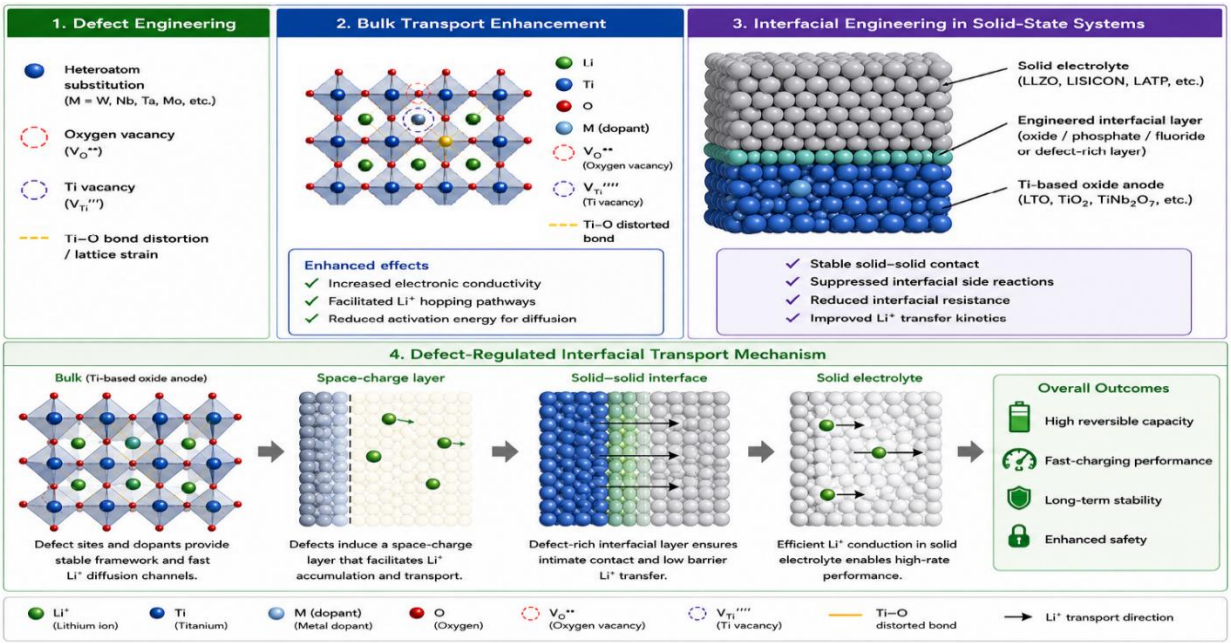

Figure 1: Defect-regulated Li^+ transport and interfacial stabilization mechanisms in titanium oxide-based solid-state battery anodes.

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Structural EPR study of a protein/single-stranded RNA condensate

Olga Vojtíšková,[1] Yinan Ni,[2] Gunnar Jeschke,[1] Frédéric Allain,[2] Maxim Yulikov[1]

[1]Department of Chemistry and Applied Biosciences, ETH Zürich, Switzerland; [2]Department of Biology, ETH Zürich, Switzerland

olga.vojtiskova@phys.chem.ethz.ch

Biomolecular condensates (BC) enriched in protein and RNA molecules are formed by liquid-liquid phase separation (LLPS). Gene expression is a common process associated with a number of membraneless organelles (cellular BCs), enriched with RNA-binding proteins (RBPs) and RNAs. New methods to investigate LLPS emerge rapidly, however, targeting structural information remains challenging. Furthermore, RBPs typically contain flexible intrinsically disordered regions which is a challenge for conventional structural biology methods. Characterization of RBPs requires integrative structural modelling approaches to determine conformational ensembles rather than a single well-defined structure. Distance distributions from DEER can be employed to restrict such a conformational ensemble in phase-separated systems.[1] In this work, we focus on polypyrimidine-tract binding protein PTBP1, a multidomain partially disordered protein, which requires RNA to phase separate. We investigate a condensate with single-stranded RNA with/without binding motifs specific for the RNA binding domains of PTBP1. The conformational distribution of dispersed PTBP1 was also investigated to identify the changes occurring after LLPS. Despite the preference of PTBP1 for specific RNA containing polypyrimidine tracts, the protein can efficiently phase separate also with non-specific RNA[2]. Structural changes to the conformational ensemble of PTBP1 have been revealed by distance distribution measurements for both types of condensates. Solvent deuteration provides proton density contrast and allows detection of changes of the local environment of a spin label due to local crowding, and thus the internal organization of BCs, using the recently developed HYSDEMON[3] methodology. These results demonstrate the potential of HYSDEMON for structural studies of LLPS systems and its compatibility with DEER. Such obtained proton density measurements can complement distance distributions and provide additional structural insights. A detailed characterization of PTBP1 structure is key for better understanding of its function in BCs. Moreover, PTBP1 plays role in various diseases, including cancer and Alzheimer's disease. The relationship between LLPS of RBPs and disease is being researched extensively.

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Electric Field Effect on Spins in Quantum Paraelectric Materials

I. Zdeg[1], O. Laguta[1], V. Laguta[2], P. Neugebauer[1]

[1] Brno University of Technology, Central European Institute of Technology, Purkyňova 656/123, 61200 Brno, Czech Republic; [2] Institute of Physics, Czech Academy of Sciences, Na Slovance 1999/2, 18200 Prague, Czech Republic

Ikram.Zdeg@ceitec.vutbr.cz

Electric-field control of magnetic properties, particularly individual quantum bits, is essential for quantum sensing and the development of logic gates in quantum computing. Traditionally, spin transitions are driven by magnetic resonance using oscillating magnetic fields. However, electric fields are easier to generate and can be confined with much higher spatial resolution, making them highly suitable for addressing individual spins. Electric-field control of spins has previously been demonstrated in quantum dot semiconductors [1], multiferroic materials [2,3], and molecular magnets [4]. In this work, we investigate iron-doped quantum paraelectric materials. Owing to their high polarizability at low temperatures, these materials are expected to exhibit strong spin–electric field coupling. We studied iron-related cubic centers using X-band electron paramagnetic resonance, with the electric field applied parallel to the magnetic field. The observed zero-field splitting shows a quadratic dependence on the electric field, yielding a spin–electric field coupling coefficient of 7.8 $Hz \cdot V^{-1} \cdot m$. Additionally, the studied single crystals exhibit high-field splitting transitions on the order of GHz. These transitions are currently being investigated using high-field, high-frequency electron paramagnetic resonance, with the aim of exploring their tunability under electric fields in different configurations.

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Probing Molecular Orientation in Surface-Confined Functionalized TEMPO Films by High-Field EPR

Muhammad Tahsin,[1] Dr. Vinicius Tadeu Santana,[1] Dr. Katarina Majerová Varga,[2] Dr. Petr Neugebauer,[1] Dr. Jiří Kaleta[2]

[1] Central European Institute of Technology, Brno University of Technology, 61200 Brno, Czech Republic; [2] Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo nám. 2, Prague 6 160 00, Czech Republic.

muhammad.tahsin@ceitec.vutbr.cz

Surface-confined organic radicals are promising platforms for molecular spin systems, but their EPR response depends not only on the number of deposited spins but also on film morphology, substrate background, and molecular orientation. Here, functionalized TEMPO films deposited on SiO_2 and Au substrates were studied by high-field EPR, supported by Raman spectroscopy, XPS, optical microscopy, SEM, and AFM. The powder spectrum was first fitted using a spin-Hamiltonian model for the TEMPO nitroxide radical (S=1/2), providing the orientation-averaged reference response of the molecule before deposition [1,2]. The drop-cast films retained the molecular vibrational and chemical fingerprints, whereas their HFEPR spectra occupied only a restricted part of the powder envelope. Orientation-distribution simulations show that the drop-cast response is dominated by the gx/gy region, while the gz-dominated part of the powder spectrum is not resolved, consistent with partial preferential orientation of the nitroxide spin centres [3]. In contrast, Langmuir–Blodgett films were confirmed on the surface by ellipsometry and PMIRRAS but did not yield a resolved molecular HFEPR signal, showing that nominal spin population alone does not guarantee EPR detectability. These results demonstrate that molecular deposition, film morphology, molecular orientation, and magnetic visibility must be considered together when designing surface-confined radical films for molecular spintronic and surface-based molecular qubit platforms [4].

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POSTER ABSTRACTS

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Self-assembly of an ultrashort peptide (Fmoc-diphenylalanine) with copper(II) into composite hydrogels

Hajar AMAL[1], H. Hashemi Haeri[1], D. Hinderberger[1]

[1] Physical Chemistry, Institute of Chemistry, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale), Germany

hajar.amal@chemie.uni-halle.de

Ultrashort peptides (USPs), built from only a few amino acids, are among the most minimal motifs that self-assemble into ordered, biocompatible nanostructures, which makes them versatile, low-cost building blocks for soft matter; coordinating metal cations to them places metal–peptide interactions at the centre of bioinorganic materials design. Fmoc-Phe-Phe (Fmoc-FF), an aromatic USP, forms β-sheet-rich, π–π-stacked supramolecular nanostructures that relate local molecular interactions to the organisation and behaviour of peptide-based soft matter.[1] Introducing Cu(II) probes how a paramagnetic transition-metal ion alters the peptide microenvironment and how buffer composition shapes the metal–peptide binding landscape.

Unlike many metal-responsive materials, peptide assemblies couple metal binding to well-defined coordination chemistry within a dynamic, reversible network formed under mild aqueous conditions, so that a single metal ion acts at once as a coordinative crosslinker and a chemical trigger. In Fmoc-FF/Cu(II) matrices, local Cu(II) binding is thus reportable through morphology and viscoelastic response, and tunable by pH, ionic strength and metal-to-peptide ratio.[2]

Building on our earlier study of Fmoc-FF with trivalent metal ions,[3] we use EPR as a site-selective reporter of the Cu(II) coordination environment: continuous-wave EPR yields the coordination geometry and hyperfine parameters, while pulsed EPR probes spatial relationships between paramagnetic centres. This is complemented by ATR-IR, TEM and rheology across water, MOPS and PBS buffers and several metal-to-peptide ratios, linking local coordination geometry to supramolecular organisation and mechanics, with calculations supporting the interpretation.

***Keywords**: Cu(II) coordination, Fmoc-FF, hyperfine spectroscopy, supramolecular hydrogels*

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EPR Immunodetection using aggregated gold nanoparticles

Stephany Natasha Arellano Ahumada[1], Luis Celedón Ornelas[1], Suset Santana Hernández[1], José Silvestre Figueroa Mendoza[2], Daniel Ramírez Rosales[1]

[1] Instituto Politécnico Nacional, ESFM, Departamento de Física, CDMX, México.
[2] Instituto Politécnico Nacional, ENCB, Laboratorio de Protección Vegetal, CDMX, México.

torchynsnat@yahoo.com.mx

Electron Paramagnetic Resonance (EPR) provides a complementary strategy for detecting antigen–antibody interactions when suitable paramagnetic probes are incorporated into the analytical system. Conventional immunoassay methods, such as ELISA, immunohistochemistry, and immunofluorescence, are widely used; however, EPR can provide sensitivity to local chemical and magnetic microenvironments. Since most proteins do not contain unpaired electrons, EPR detection requires a probe whose signal changes upon antigen–antibody recognition.

In this work, aggregated gold nanoparticles (AuNPs) deposited on a non-paramagnetic cellulose-based substrate were evaluated as EPR-active probes for antigen–antibody detection. AuNPs are attractive for analytical applications because of their reproducible synthesis, environmental sensitivity, and size-dependent magnetic properties. Previous studies have reported EPR immunoassays using iron oxide nanoparticles as probes[1], while magnetic ordering has also been observed in gold nanoclusters[2].

To avoid water-related interference in EPR measurements, AuNP suspensions were filtered and deposited onto cellulose-mixed filters. Different aggregation states were induced by varying the salt concentration during deposition. The resulting substrates exhibited detectable EPR signals, supporting their use as solid-supported probes. The AuNP-coated substrates were then functionalized with bovine serum albumin (BSA) as a model antigen and exposed to anti-BSA antibody solutions under controlled chemical conditions.

The analytical response was assessed by monitoring changes in the EPR spectrum, including signal shifts and intensity variations, as a function of antigen and antibody concentration. These results were compared with non-reactive control systems. This EPR-based platform provides a promising route for detecting antigen–antibody reactions and may contribute to the development of alternative immunoassay protocols for human, veterinary, and plant pathology diagnostics.

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Spin echo studies in ZnO:Mn^{2+} under conditions of high electron spin polarization

D.V. Azamat[1], L. Jastrabik[2], M. Fanciulli[3], A. Dejneka[2], D.R. Yakovlev[1], and M. Bayer[1, 4]

[1] Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany; [2] Institute of Physics of the Czech Academy of Sciences, 182 21, Prague 8, Czech Republic; [3] Department of Chemistry, University of Torino, Via P. Giuria 9, 10125 Torino, Italy; [4] Research Center FEMS, Technische Universität Dortmund, D-44221 Dortmund, Germany

e-mail dmitry.azamat@tu-dortmund.de

Nonlinear effects were observed in some paramagnetic systems. The suitable system for maser applications might be Mn^{2+} in ZnO co-doped with the faster relaxer like Co^{2+}. In the present study we describe the measurements on Mn^{2+} system in hydrothermally grown ZnO. The applicability of ZnO:Mn^{2+} system for solid state optically pumped maser amplifiers is under consideration.

The optically pumped EPR spectrum of ZnO:Mn^{2+} system demonstrates the selectivity in the population of the manganese electron-nuclear spin levels. The cross-relaxation give rise to the process of dynamic nuclear polarization of ^{55}Mn in this system. The time dependent inversion of the populations for Mn^{2+} electron-nuclear states has been observed when applying the optical pumping below 3 K.

The thermal mixing DNP process taken in the high temperature approximation involves a spin system broken up into several heat reservoirs with different spin temperatures: the electron Zeeman, the nuclear Zeeman, and the spin-spin interactions reservoirs. The electron spectral diffusion is studied under dynamic nuclear polarization by using electron spin-echo-detected EPR spectra and Electron-Electron Double Resonance (ELDOR) technique in heavily cobalt doped ZnO:Mn^{2+} at the Co^{2+} exchange narrowing temperature range. It is established that the thermal mixing mechanism of DNP leads to the cooling of the common reservoir of electron dipole-dipole interactions of Mn^{2+} and Co^{2+} spins to the single spin temperature in the rotating frame. We show the variation of the polarization amplification of the common nuclear subsystem as a function of microwave irradiation frequency.

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Investigating conformational equilibria and ligand binding using cw-EPR spectroscopy

Martin Buhlmann[1], Ivan Yushin[1], Anna L. Krauspe[1], Dilara Öğütcü[1], Matthias Elgeti[1,2]

[1] Institute for Drug Discovery, Institute for Medical Physics and Biophysics, University of Leipzig Medical School, Germany; [2] Integrative Center for Bioinformatics, University of Leipzig, Germany

martin.buhlmann@medizin.uni-leipzig.de

Electron paramagnetic resonance (EPR) spectroscopy in combination with site-directed spin labeling (SDSL) presents a versatile method for studying the structure and dynamics of biomolecules[1]. In particular, continuous wave EPR (cw-EPR) is a powerful tool to evaluate nanosecond dynamics and conformational heterogeneity qualitatively and quantitatively. Here, we present a cw-EPR method for determining dissociation constants (K_D) of ligand binding. Because cw-EPR's limited sensitivity requires protein concentrations often exceeding the affinity to be determined, ligand depletion during titration becomes non-negligible, making K_D-estimates unreliable[2]. We circumvent this limitation by utilizing solid-support attachment, demonstrated for the Maltose Binding Protein (MBP) and Calmodulin. For Calmodulin, we additionally observe different binding behavior depending on the label site, reflecting its multiple, non-equivalent Ca^{2+}-binding sites and demonstrating that our approach is site-sensitive. Our goal is to apply these methods to more complex systems such as G-protein coupled receptors (GPCRs), establishing cw-EPR as a site-resolved conformational biomarker for pharmacological profiling[3].

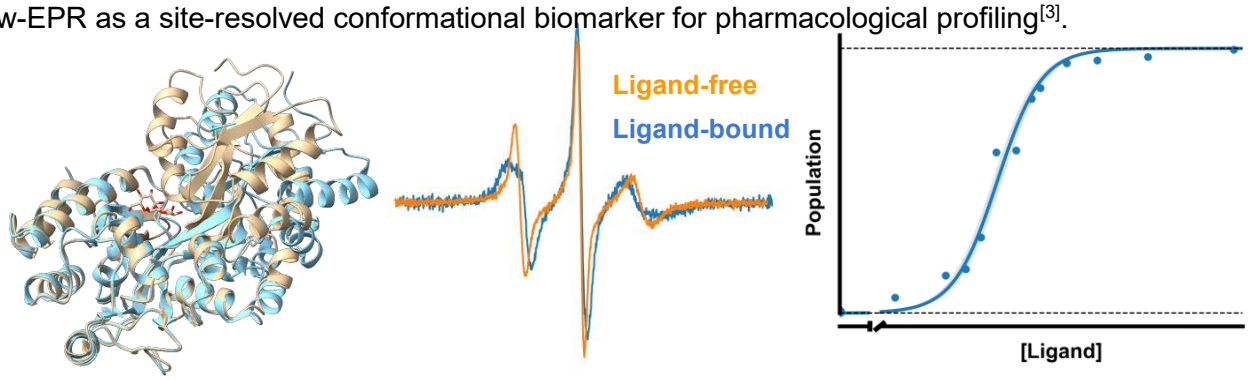

Figure 1: Upon binding its endogenous ligand maltose, the Maltose Binding Protein undergoes a conformational change. The spin label's altered environment is reflected in a changed cw-EPR spectrum, which allows state-specific quantification.

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EPR characterization of interactions between RNA-binding proteins SRSF1 and hnRNP A1

Camille Camescasse,[1] Laura Galazzo,[1] Elise Komarczuk,[1] Noémie Kociolek,[2] Rajika Arora,[2] Maxim Yulikov,[1] Frédéric Allain,[2] Gunnar Jeschke[1]

[1] Department of Chemistry and Applied Bioscience, Institute for Molecular Physical Sciences, ETH Zürich, Switzerland; [2] Department of Biology, Institute of Biochemistry, ETH Zürich, Switzerland.

camille.camescasse@phys.chem.ethz.ch

RNA-binding protein systems are increasingly recognized as central players in a wide range of neurological and pathological diseases.[1] Spinal Muscular Atrophy (SMA) is no exception, as a neuromuscular disease involving two gene regulators: hnRNP A1 (Heterogeneous Nuclear Ribonucleoprotein A1) and SRSF1 (Serine/arginine-Rich Splicing Factor 1). These biomolecules are involved in the transport, maintenance and regulation of RNA, and are well known for their antagonist splicing activity of the *SMN* (Survival of Motor Neuron) gene,[2] whose protein product is crucial for preserving motor neuron health. HnRNP A1 and SRSF1 present a very similar structural organization; both contain two RRMs (RNA-Recognition Motifs), connected via a flexible linker, and a disordered C-terminus tail (Intrinsically Disordered Domain, IDD).

Understanding the structure and dynamic properties of these RNA-binding proteins has been revealed crucial to understanding their mode of action. However, their lack of a well-structured three-dimensional fold and their tendency to undergo Liquid-Liquid Phase Separation (LLPS) make their investigation via conventional structural biology techniques extremely challenging, highlighting EPR as an attractive alternative for probing their conformational ensembles.[3]

This study aims to investigate the interactions between hnRNP A1 and SRSF1 using EPR. Four-pulse DEER was used to investigate the effect of SRSF1 on different intramolecular distances of hnRNP A1. Sample preparation and mixing conditions were first optimized, confirming that SRSF1's urea-containing storage buffer does not perturb hnRNP A1 folding. Distance measurements for several intra-hnRNP A1 spin-label pairs were established in the presence of SRSF1, under dispersed or LLPS conditions. These experiments are expected to provide initial structural insights into how their interaction relates to SMA-associated splicing regulation.

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Hydrogen isotope adsorption in V-doped MIL53(Al) via *in-situ* EPR spectroscopy

Pranjit Das[1], Andreas Pöppl[1*]

[1]Felix-Bloch-Institute of Solid-State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, Linnéstrasse 5, Leipzig 04103, Germany

pranjit.das@uni-leipzig.de

Metal-organic frameworks (MOFs) are well explored for their tunable properties like gas storage, band gap, catalysis, etc. Among them, flexible MOFs such as MIL53(Al) exhibits selectivity towards hydrogen isotope adsorption and separation at low temperature[1]. In this study, a vanadium-doped variant of MIL53 (Al) has been considered where the V^{4+} ions acts as paramagnetic probes to monitor the local structural change in the framework upon adsorption of molecular hydrogen. The *in-situ* EPR spectroscopy clearly detect the presence of the narrow-pore (NP) and the large-pore (LP) phase for both hydrogen (H_2) and deuterium (D_2) isotopes, and notably an additional very-large-pore (VLP) phase that is only visible for D_2 adsorption at low temperatures[2]. These findings demonstrates that such a system provides a sensitive platform for probing hydrogen isotope adsorption and separation. Further understanding such adsorption processes could potentially contribute to the application of gas molecules separation and storage using metal-organic frameworks.

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Synthesis and Structural Characterization of a Heteroleptic Copper(II) Complex Based on L-phenylalanine

Pedro H. O. Santiago,[1] Daina Arenas,[1] Vinicius T. Santana[1]

[1] Central European Institute of Technology, Brno University of Technology, Brno, 61200, Czech Republic

santiago@vutbr.cz

Transition metal complexes are promising candidates for new magnetic materials with potential applications as single-molecule magnets and quantum bits[1,2,3]. The advantage of molecular compounds lies in their diverse and adjustable geometries, resulting in tunable magnetic properties via synthetic routes. In this context, understanding magneto-structural correlations is fundamental to the design of new complexes. Building on a previous study correlating structure and magnetic exchange interactions[4], we report the characterization of a new Cu(II) complex with L-phenylalanine and 2,2'-bipyridine, [CuCl(L-Phe)(bipy)], using single-crystal X-ray diffraction and spectroscopic techniques. The complex has a distorted square pyramidal geometry, and crystallized in the non-centrosymmetric monoclinic space group $P2_1$, composed of two crystallographically independent molecules of the pentacoordinated complex [CuCl(L-Phe)(bipy)] in the asymmetric unit (Z' = 2), which differ in the orientation of the phenyl group of L-Phe (Figure 1). Based on Hirshfeld surface analysis, we identified a plausible pathway for weak intermolecular exchange between neighboring Cu(II) centers[4], which is currently being investigated using high-field EPR (HFEPR) to extract the corresponding coupling parameters.

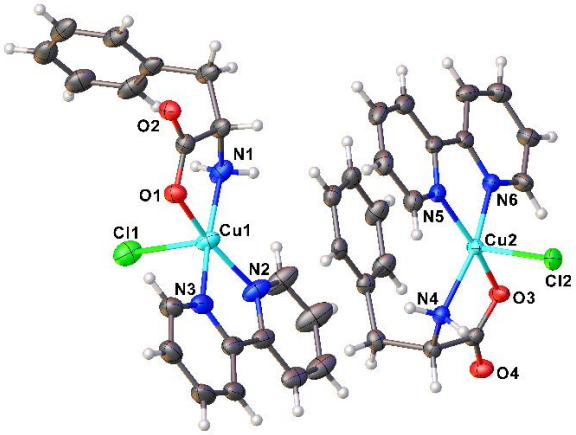

Figure 1: ORTEP type illustration of the asymmetric unit of [CuCl(L-Phe)(bipy)].

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EFEPR 2026 CONFERENCE
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Paramagnetically Doped Metal–Organic Frameworks for Dynamic Nuclear Polarization: An EPR Study

Antareekshya Deka,[1] Andreas Pöppl,[1]

[1]Felix-Bloch-Institute of Solid-State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, Linnéstrasse 5, Leipzig 04103, Germany

antareekshya.deka@uni-leipzig.de

Metal-Organic frameworks (MOFs) have recently emerged as promising materials for gas storage and separation due to their high surface areas, high porosity, framework flexibility, etc [1,2]. MOFs are highly tunable porous materials with large surface areas, high porosity, and structural flexibility, enabling applications ranging from gas storage, separation, catalysis, etc [1,2]. Unlike rigid porous solids, many MOFs undergo dynamic structural transformations such as breathing, gate-opening, or swing effects in response to guest adsorption, temperature, or pressure [2-4].

In this work, Electron Paramagnetic Resonance (EPR) spectroscopy was employed to characterize a well-known MOF: MOF-76(Y), an activated yttrium metallic–organic framework of 1,3,5-benzenetricarboxylate, and to investigate its guest adsorption behavior. To gain insight into the local environment of the MOF-76(Y) framework and its host–guest interactions, high-spin paramagnetic metal ion like Gd^{3+} (S=7/2) was introduced as spin probes into the framework. Such S-state ions (with minimal orbital angular momentum) are particularly well-suited for Dynamic Nuclear Polarization (DNP) due to their suitable electron relaxation times and efficient polarization transfer, making them ideal candidates for hyperpolarization studies in solid-state NMR [5,6]. The insights gained from this research will provide a deeper understanding of MOF materials doped with high spin metal ion centers and will also emphasize their potential for practical applications like gas adsorption, gas separation, and hyperpolarization techniques. Together, these approaches contribute to establish MOFs as versatile platforms for probing framework dynamics and developing next-generation DNP strategies for hyperpolarization of adsorbed gases or guest molecules in porous materials.

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Field-free spin wave dynamics in stripe magnetic domains

Anuj K. Dhiman[1 #], Nikodem Lesniewski[1], Ryszard Gieniusz[2], Jan Kisielewski[2], Piotr Mazalski[2], Zbigniew Kurant[2], Michał Matczak[3], Feliks Stobiecki[3], Maciej Krawczyk[2], Artem Lynnyk[4], Andrzej Maziewski[2], Paweł Gruszecki[3]

[1] Faculty of Physics and Astronomy, Adam Mickiewicz University, Poznan, Poland; [2] Department of Physics of Magnetism, University of Bialystok, Bialystok, Poland; [3] Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland; [4] Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

[#]*dhiman@ifmpan.poznan.pl*

Controlling spin-wave (SW) propagation typically relies on external stimuli such as magnetic fields, electric currents, or sophisticated nanopatterning approaches, all of which become increasingly difficult to implement at the deep nanoscale. In this work [1], we address these challenges by demonstrating SW propagation in Pt/Co multilayers at remanence, where the propagation is governed by stripe domain patterns. We show that stripe domains with a periodicity of approximately 100 nm are readily reconfigurable: their orientation can be rotated using an in-plane magnetic field while preserving their morphology. This reconfigurability enables the investigation of SW propagation both perpendicular and parallel to the stripe domains. Distinct multimode SW spectra are observed, comprising three bands for the perpendicular configuration and five bands for the parallel configuration. Micromagnetic simulations reproduce the experimental results, allowing all observed modes to be identified and revealing that the differences between the two geometries arise from the varying contributions of the three magnetization components to the SW dynamics. Furthermore, we demonstrate the experimentally observed nonreciprocal dispersion for wavevectors perpendicular to the stripes resulting from an asymmetric intensity of two low-frequency modes. These findings establish stripe-domain-engineered Pt/Co multilayers as a promising platform for reconfigurable and energy-efficient nanomagnonic devices.

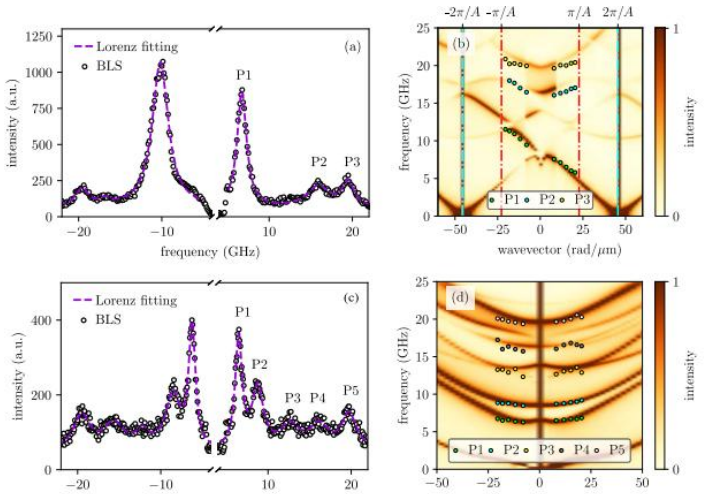

Figure 1 SW propagation in a stripe domain structure in the remanent state. (a) and (c) The experimental BLS spectra (black circles) measured for k perpendicular and parallel to stripes, respectively. (b) and (d) Simulated band structure with experimental data points for *k* perpendicular and parallel to stripes.

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Graphene Quantum Dots Coated with a Cobalt (II)-Based Single-Ion Magnet for Electrical Detection of Magnetization Switching

Djaba Paul Vianel[1], Mohamed Amine Rhanbouri[1], Oleh Martyniuk[2], Ivan Nemec[2,4], Ondřej F. Fellner[4], Muhammad Tahsin[2], Paola Barbara[3], Petr Neugebauer[2], Abdelouahad El Fatimy[1]

[1] College of Physical Sciences and Engineering, Mohammed VI Polytechnic University, Ben Guerir, 43150, Morocco; [2] Central European Institute of Technology, Brno University of Technology, Purkyňova 656/123, 61200 Brno, Czech Republic; [3] Department of Physics, Georgetown University, Washington, DC 20057, USA; [4] Department of Inorganic Chemistry, Faculty of Science, Palacký University, 17. listopadu 12, 77147 Olomouc, Czech Republic.

paul.vianel-djaba@um6p.ma

Molecular spintronics is based on electronic components functionalized with magnetic molecules, specifically single-molecule magnets, so that molecular spin states control the transport of electrons through the device [1,2]. In this work, we deposited a cobalt (II)-based single-ion magnet [3] onto a device consisting of three quantum dots arranged in parallel to manipulate and electrically read the spin states of Co (II) complex [4]. The results show that the electrical response associated with molecular magnetization switching depends strongly on source–drain bias voltage. We also found that applying a magnetic field significantly increases the relaxation time, confirming the designation of a field-induced single-ion magnet. X-ray photoelectron spectroscopy measurements showed that the solvent has no effect on the core-level binding energies of the atoms comprising the complex. Furthermore, despite the application of 7 T magnetic fields, the molecules deposited by drop-casting remain attached to the surface, thus demonstrating their stability on the graphene quantum dot surfaces. These results are promising and pave the way for further investigations into these cobalt (II)-based single-ion magnets coupled to quantum dots, with the aim of enhancing numerous applications in molecular spintronics.

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Fluorinated Nitroxide-Functionalized Hydrazone Switches as Potential Stimuli-Responsive dual ^{19}F MRI/EPR Probes

Eliška Dolejšová,[1,2 *] Ivan Nemec,[1,3] Vinicius T. Santana,[1] Lucie Kotásková[1]

[1] Central European Institute of Technology, Brno University of Technology, Purkyňova 656/123, 61200 Brno, Czech Republic; [2] Department of Chemistry, Faculty of Science, Masaryk University, Kotlářská 267/2, 611 37 Brno, Czech Republic; [3] Department of Inorganic Chemistry, Faculty of Science, Palacký University, 17. listopadu 12, 77900 Olomouc, Czech Republic

**eliska.dolejsova@ceitec.vutbr.cz*

Hydrazone-based molecular switches represent versatile platforms for responsive materials due to their multi-stimuli isomerization and high thermal stability.[1] This work examines two fluorinated (−F or −CF_3) nitroxide-functionalized hydrazones (Figure 1) as metal-free ^{19}F MRI and EPR probe alternatives to widely used gadolinium counterparts.[2] Successful pH- and partial photo-induced isomerization was confirmed for both compounds (using UV–Vis and NMR spectroscopy), while EPR spectroscopy verified that no degradation occurred during the process. The photo-induced isomerization alters the distance between the nitroxide radical and the ^{19}F nucleus, leading to changes in relaxation time values (Figure 1). By combining photoswitching with paramagnetic relaxation, this work demonstrates the controllable modulation of ^{19}F NMR relaxation times. These findings establish nitroxide-functionalized hydrazones as versatile, metal-free, stimuli-responsive dual ^{19}F MRI/EPR probes, with potential for extension into surface-deposited, photoswitchable arrays for molecular magnetism.[3]

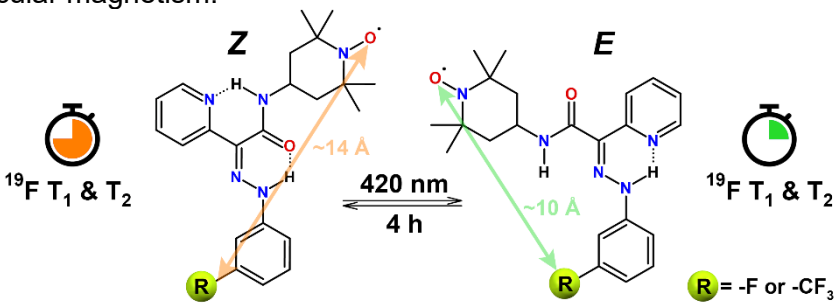

Figure2: Modulation of ^{19}F relaxation times via photoswitchable distance changes in fluorinated nitroxide hydrazones.

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Probing Self-Assembled Prebiotic Structures via Spin-Probe EPR

Daniele Dondi,[1] Dhanalakshmi Vadivel,[1] Yishi Ezerzer,[2] Moran Frenkel-Pinter[2]

[1] Department of Chemistry, University of Pavia, Viale Taramelli 12, 27100 Pavia, Italy;

[2] Institute of Chemistry, The Hebrew University, Givat Ram Campus, Jerusalem 91904 Israel;

daniele.dondi@unipv.it

Wet–dry cycling of hydroxy acid and amino acid mixtures provide a plausible prebiotic route to functional oligomers [1]. In this work, conducted in collaboration with Moran Frenkel-Pinter's Chemical Evolution Laboratory, we systematically investigated binary and ternary mixtures subjected to dehydration under thermal conditions (85 °C for 1 week), either in the absence or in the presence of additional UVC irradiation. The resulting complex ensembles of oligomers and co-polymers were characterized by using 1D/2D NMR spectroscopy, HPLC-MS, and, in an innovative extension, continuous-wave X-band EPR. EPR spectroscopy was employed to probe the micro viscosity of vesicles and self-assembled structures formed upon dispersing the reaction residues in solvent/non-solvent systems. Motion-sensitive 16-doxyl radical spin probes enabled temperature-dependent measurements of local mobility, revealing pronounced differences between irradiated and thermally processed samples. Notably, UVC-treated products containing phenyl moieties exhibited significantly reduced probe mobility, suggesting tighter packing or altered supramolecular organization within the resulting vesicles. These findings indicate that UVC irradiation not only modulates the chemical composition of prebiotic oligomers but also impacts the physical properties of their self-assembled compartments, with potential implications for protocellular dynamics and early compartmentalization processes.

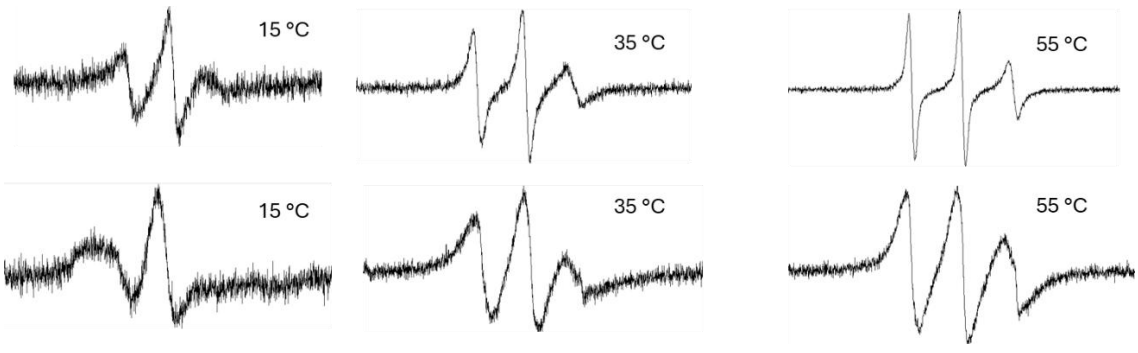

Figure 1: Spin probe measurement of a mixture of phenyl lactic acid and glycine at different temperature. Top: thermal treatment only; Bottom: concomitant UVC treatment.

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Beyond Spin Trapping: Reliable Reactive Species Identification in (Photo)Catalysis

Dana Dvoranová,[1] Sridhar Gowri Sankaran,[1,2] Olivier Monfort[2]

[1] Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic; [2] Department of Inorganic Chemistry, Faculty of Natural Sciences, Comenius University Bratislava, Ilkovičova 3278/6, SK-841 04 Bratislava, Slovak Republic

dana.dvoranova@stuba.sk

Advanced oxidation processes (AOPs) based on metal oxides, metal-organic frameworks (MOFs), and their hybrids are widely investigated for environmental remediation and sustainable energy applications. Owing to its sensitivity towards paramagnetic intermediates, X-band electron paramagnetic resonance (EPR) spectroscopy has become the standard analytical tool for mechanistic studies of these systems. Since most reactive oxygen species (ROS) are extremely short-lived, their identification relies predominantly on indirect EPR methodologies. The widespread use of indirect EPR has significantly advanced the understanding of (photo)catalytic mechanisms but has also revealed frequent overinterpretation of EPR data. In complex catalytic systems, multiple radical and non-radical pathways coexist, while spin-trap selectivity is often overestimated, leading to questionable reactive species assignments and misleading mechanistic conclusions. Attention is devoted to peroxymonosulfate (PMS) activation, where DMPO remains the benchmark spin trap. DMPO- and BMPO-derived spin adducts are critically compared, with emphasis on the interpretation of the $^{\bullet}$BMPO-SO_4^{-} spin-adduct and the limitations of reactive species assignment in complex reaction networks. Critical interpretation of indirect EPR data, supported by complementary experimental evidence, is essential for reliable reactive species identification and the rational design of next-generation (photo)catalysts [1-3].

Acknowledgement

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Artificial intelligence tools were used in the preparation of this abstract (for language editing and stylistic refinement).

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Synthesis and Structural Characterization of Layered Na-Ni-Mn Oxides for Sodium-Ion Batteries Using Sol-Gel Precursors

Dominika Działkowska[1], Marcin Godzierz[2], Małgorzata Czichy[1,3], Paweł Czulkin[1,3], Vinicius Tadeu Santana[4], Daina Dayana Arenas Buelvas[4], Yauhen Aniskevich[3]

[1] Silesian University of Technology, Gliwice, Poland; [2] Centre of Polymer and Carbon Materials PAN, Zabrze, Poland; [3] Silesian University of Technology, Centre for Organic and Nanohybrid Electronics (CONE), Gliwice, Poland; [4] Central European Institute of Technology (CEITEC), Brno, Czech Republic

dd309877@student.polsl.pl

Sodium-ion batteries are considered a promising alternative to lithium-ion batteries due to the high abundance and low cost of sodium resources. Among the investigated cathode materials, layered transition-metal oxides, particularly Na-Ni–Mn-based compounds, have attracted considerable attention due to their structural flexibility and promising electrochemical properties. The aim of this study was to synthesize $Na_{0.67}Ni_{0.33}Mn_{0.67}O_2$ and $Na_{0.7}[Li_{0.1}Mg_{0.05}Ni_{0.15}Mn_{0.7}]O_2$ using a sol–gel precursor route. The materials were characterized by X-ray diffraction (XRD) and X-band electron paramagnetic resonance (EPR) spectroscopy to investigate the correlation between structural-magnetic properties and how it impacts the electrochemical performance of the batteries. Rietveld refinement of XRD results confirmed the formation of a layered hexagonal P2-type structure characteristic of sodium transition-metal oxides and EPR measurements were used to investigate paramagnetic centers associated mainly with manganese ions and to provide information on their local electronic environment. The synthesized materials were subsequently evaluated as cathode active materials in sodium-ion batteries using galvanostatic charge–discharge measurements to assess their electrochemical properties and cycling behaviour. The results contribute to a better understanding of these materials and their potential application as cathodes for sodium-ion batteries.

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Broadband Pulse High Field EPR spectroscopy

Amirmohsen Fanisaberi,[1] Oleksii Laguta,[1] Petr Neugebauer[1]

[1] CEITEC, Central European Institute of Technology, Brno University of Technology, Brno, Czech Republic

Amirmohsen.Fanisaberi@ceitec.vutbr.cz

Pulsed operation of high-field / high-frequency EPR remains experimentally demanding. Here we report progress toward pulsed HF-EPR on our quasi-optical spectrometer, which covers 95 GHz to 1.1 THz in magnetic fields of up to ±16.1 T. A variable-temperature insert (VTI) with a 50 mm bore allows measurements from 1.8 K to 320 K. Dedicated sample holders accommodate solids, liquids, oriented single crystals (three rotation planes), and chips[1] for CW-EPR and frequency-sweep rapid scan measurement.

For pulsed experiments, a Fabry–Pérot resonator was built with photolithographic mesh on cover glass (22 µm thickness) and a concave mirror, providing a high Quality Factor. Tuning and coupling inside the VTI are controlled with a piezo nanopositioner of 100 nm. The sample can be placed on the mirror to maximise the microwave magnetic field, or on the mesh to maximise power; the mesh coating can be conductive (gold) or non-conductive (SiO_2). The same sample holder supports continuous-wave EPR with field modulation of up to 10 G as well as pulsed HF-EPR. Superheterodyne detection recovers the time-domain response with the required bandwidth and sensitivity. Due to cross polar measurement, there is no need to protect the detectors, which enables access to ultra-fast relaxation times. Building on this platform, we implement pulsed excitation and arbitrary-waveform generation for time-shaped microwave pulses, aiming at broader excitation bandwidth, reduced resonator ringing, and flexible high-frequency.

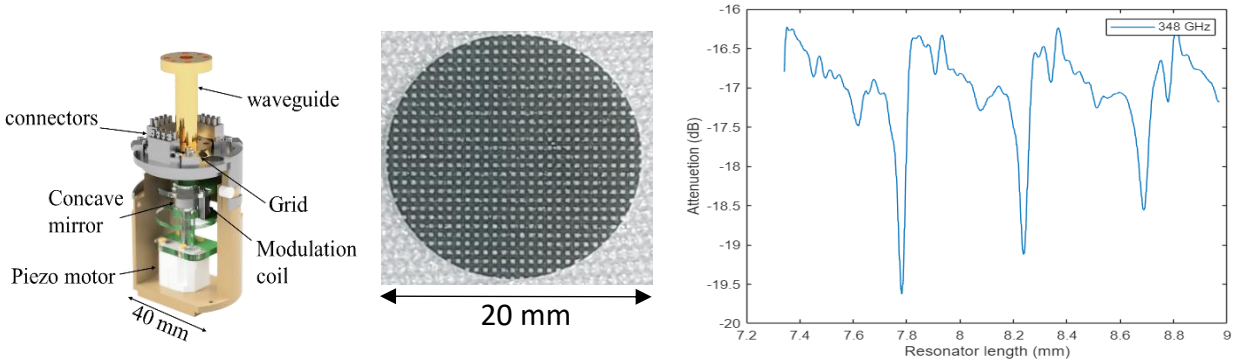

Figure 1: (Left) Pulse HFEPR sample holder, (Middle) semi-transparent mesh, (Right) Resonator reflection

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DYNAMIC YET DEFINED – SELF-ASSEMBLY OF SMALL MOLECULES IN SOLUTION: COLLOID-LIKE IONIC CLUSTERS (IONOIDS).

Daylin Fernández Pacheco,[1] Anna Franziska Roth[1], Dr. Haleh Hashemi Haeri[1], Prof. Dr. Dariush Hinderberger[1]

[1] Martin-Luther-University Halle-Wittenberg, Institute of Chemistry, Physical Chemistry – Complex Self-Organizing Systems, Halle (Saale), Germany.

daylin.fernandez-pacheco@chemie.uni-halle.de

In the search for new polymers based on non-covalent molecular forces, a new class of colloidal ionic clusters, known as "ionoids," was discovered in 2012.[1] These structures consist of a multicationic molecular cage, such as the "Texas-sized molecular box"[2], combined with a dianionic salt, such as dipotassium methanedisulfonate (MDS) or Fremy's salt. Ionoids are spherical, monodisperse structures with a hydrodynamic radius ranging from 6 nm to 8 nm, characterized by remarkable stability.[3] Their self-assembly occurs spontaneously under specific solvent conditions (DMSO:glycerol:water in a 50:43:7 v/v/v ratio) after an incubation period of ten days at room temperature. This self-assembly process results from a combination of factors, including preferential solvation, viscosity, van der Waals interactions, and long-range correlated electrostatic forces.[4]

In this work, we report the synthesis of a "Texas-sized molecular box" and two other macrocycles through a macrocyclization reaction combining a common linker and two different heterocyclic heads. The initial stages of the ionoids derived from these two macrocycles and Fremy's salt as spin probe, have been analyzed by means of electron paramagnetic resonance (EPR) spectroscopy. In addition, the properties of the ionoids derived from the two macrocycles and dipotassium methanedisulfonate (MDS), such as the forces and mechanisms governing their formation and stability, have been studied using dynamic light scattering (DLS). The preparation of new linkers, heterocyclic heads, macrocycles, and ionoids is underway. Stay tuned for further results!

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Development and Optimization of Probeheads for MAS-EPR Spectroscopy

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

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

fialkov@tauex.tau.ac.il

Pulsed Electron paramagnetic resonance (EPR) is the only spectroscopic method to provide direct access to electron spin dynamics governing Dynamic Nuclear Polarization (DNP). However, conventional EPR experiments are performed on static samples at relatively low magnetic fields, whereas modern DNP operates under magic angle spinning (MAS) at high magnetic fields. This motivated the development of dedicated MAS-EPR instrumentation capable of probing electron spin dynamics under DNP-relevant conditions.

Over the past several years, we have developed and tested two complementary high-field MAS-EPR probehead architectures integrated with a dual 7 T / 14 T EPR-DNP spectrometer [1]. The first design was based on the spherical rotor concept introduced by the Barnes group [2] and enabled the first high-field pulsed MAS-EPR experiments. The second design employed a modified PhoenixNMR MAS-DNP probehead, extending MAS-EPR operation to spinning frequencies up to 37 kHz and enabling rotor-synchronized experiments.

Unlike MAS-DNP, where efficient transmission of a single linearly polarized mm-wave mode is sufficient, induction-mode MAS-EPR requires efficient propagation of two orthogonal mm-wave polarizations for excitation and signal detection. The solenoid RF coil surrounding the rotor in the PhoenixNMR acts as a wire grid polarizer therefore introducing a fundamental compromise between mm-wave transmission efficiency and preservation of the receive polarization. Despite this expected limitation, we were able to achieve efficient mm-wave mm wave coupling efficiency of both transmitted and received signals leading to an improved, B1 fields and superior signal-to-noise ratio.

These results provide practical design guidelines for future MAS-EPR and MAS-DNP instrumentation and demonstrate that careful optimization of mm-wave propagation is essential for efficient EPR experiments under MAS conditions.

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LISTENING FOR SPINS: PHOTOACOUSTIC EPR

Laisvydas Giriūnas,[1] Gediminas Usevičius[1], Vidmantas Kalendra[1], Jūras Banys[1] and Mantas Šimėnas[1]

[1] Faculty of Physics, Vilnius University, Sauletekio av. 9, 10222 Vilnius, Lithuania

laisvydas.giriunas@ff.vu.lt

We present photoacoustic electron paramagnetic resonance (PA EPR) as a method to detect EPR spectra from paramagnetic and ferromagnetic particles suspended in liquids. Resonant microwave absorption produces nonradiative heating that drives periodic thermal expansion of the liquid and launches acoustic waves [1], which are detected by a submerged microphone. We demonstrate this approach using an X-band resonator filled with benzene and an immersed waterproof microphone; microwaves are applied while an external magnetic field is swept and the modulated acoustic signal is recovered with a lock-in amplifier [2]. Using Ni–Zn ferrite suspended in benzene, PA EPR produced clear resonance peaks that match conventional CW-EPR, demonstrating reliable acoustic detection of spin resonances in liquid. Ongoing work will quantify sensitivity limits and optimize coupling and microphone placement.

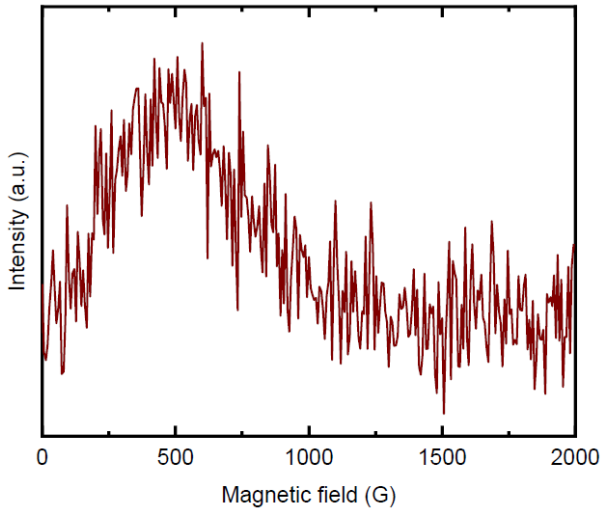

Figure 1: Photoacoustically detected EPR spectrum of Ni-Zn ferrite with benzene as a transducer liquid.

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Spin-echo interferometry in paramagnetic defect-based qubits

Suraj Halder,[1] Sheetal Kumar Jain,[1]

[1] Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru, India

surajhalder@iisc.ac.in

Hybrid systems consisting of an electron spin interacting with nearby nuclear moments are widely used in quantum sensing, quantum computing, and dynamic nuclear polarization (DNP)—with key examples being NV^- centers in diamond and VB^- centers in h-BN. In these systems, the transverse component of an external magnetic field mixes the spin states, causing an envelope modulation of the electron spin echo intensity over time.[1] However, the role of the pseudo-secular part of hyperfine coupling is often ignored in calculations determining the envelope modulation frequencies in the optical detection of the defect qubit systems.[2,3] Our calculations show that the pseudo-secular hyperfine component significantly alters the nuclear precession frequency in spin-1 electronic systems while heavily enhancing nuclear sensitivity, as shown in Figure 1. We provide the analytical theory using the Schrieffer-Wolff (SW) transformation, a unitary transformation technique to find the effective Hamiltonian. We further compare theoretical and numerical results to investigate the effects of microwave pulses, such as Electron Spin Echo and Ramsey, in the presence of single or multiple coupled nuclei. Especially near the ground state level anti-crossings (GSLAC), the effect is a bit more complex due to the degeneracy in the $|0\rangle$ and $|-1\rangle$ levels and needs to be explained using degeneracy theory. In general, NMR, ESR, and DNP detection in such systems can utilize this theoretical model for core understanding and for application to gyroscopic and AC-field sensing.

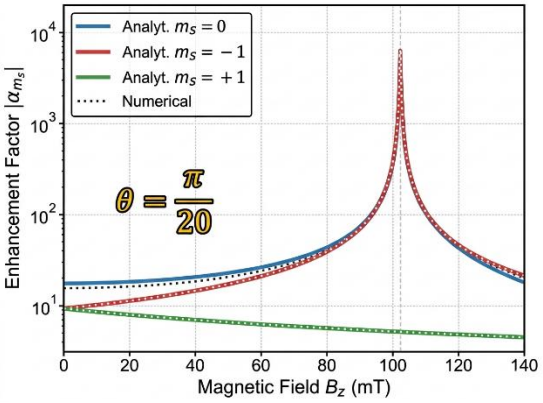

Figure 1: Enhancement of the nuclear Larmor frequency with a magnetic field along z and to the different m_s states. Also. Compared with the numerical data.

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New Approaches for Force Field parametrization of amino acid residues containing unpaired electrons

Ivan Iushin,[1] Matthias Elgeti[1,2]

[1] Leipzig University Medical School, Institute for Drug Discovery and Institute for Medical Physics and Biophysics, Leipzig, Germany; [2] Leipzig University, Integrative Center for Bioinformatics, Leipzig, Germany

ivan.iushin@uni-leipzig.de

The methods of electron paramagnetic resonance (EPR) play an important role in the fields of structural biology and biophysics. The pulsed EPR techniques, such as DEER/PELDOR and RIDME can provide the distance distribution between the spin centres. Molecular dynamics (MD) simulations can be used to predict theoretical distance distributions using all-atom models of the protein and spin labels. The simulated spin-spin distance probability can be used to accurately interpret EPR distance distributions and relate them to protein structure and dynamics. However, the application of MD simulation is limited by the lack of force-field parameters for many non-standard amino acids.

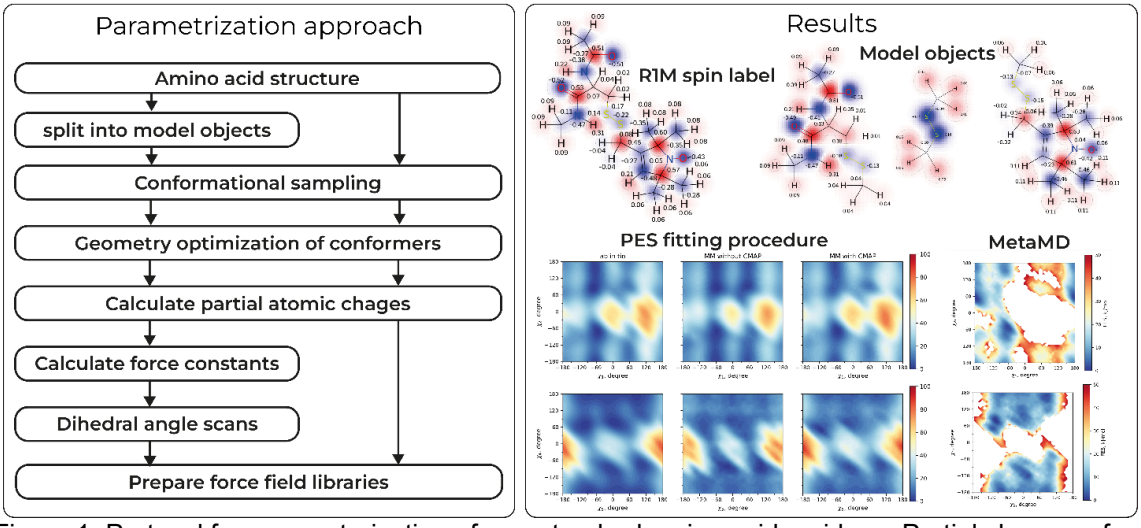

Figure 1: Protocol for parameterization of non-standard amino acid residues. Partial charges of amino acid and model fragments. PES obtained using QM and MM methods. Potential energy surface calculated from an MD simulation.

Here we present an approach for development and validation of force-field parameters for non-standard amino acid residues containing unpaired electrons (Figure 1). This approach extends the applicability of molecular dynamics simulations in combination with pulsed EPR techniques, allowing more accurate prediction and interpretation of spin-spin distance distributions and providing deeper insight into protein structure and dynamics.

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EPR spectroscopy as a versatile tool for the characterization of ultra-short peptide materials

Melissa Kemesies,[1] Haleh H. Haeri,[1] Dariush Hinderberger[1]

[1]Martin Luther University Halle-Wittenberg, Institute of Chemistry, Physical Chemistry, Faculty of Natural Sciences II, Von-Dankelmann-Platz 4, 06120 Halle (Saale), Germany

melissa.kemesies@student.uni-halle.de

Peptides continue to attract growing interest, both as novel therapeutic agents and as building blocks for pharmaceutical materials like hydrogels. Due to their structural simplicity, biocompatibility and ease of synthesis[1], ultra-short peptides (<7 amino acids[2]) are of particular interest. Through the study of two representative peptide systems, we demonstrate EPR spectroscopy as a powerful analytical method for structural and dynamic characterization.

The dipeptide Fmoc-Diphenylalanine (FmocFF) served as a representative system for peptide hydrogelators with a potential for drug delivery. We performed CW-EPR spin-probing experiments to investigate different aspects of molecular-level organization within the hydrogel network. The spin probes were found to occupy different regions of the hydrogel, depending on their structure and interaction with Fmoc-FF[3]. The resulting insights into network polarity and non-covalent interactions provide a basis for evaluating drug compatibility with FmocFF-based delivery systems.

We further tuned the hydrogel structure with different physiologically relevant metal cations (Cu^{2+}, Fe^{3+}, Al^{3+})[3]. The combination of both transition-metal EPR and spin-probing yielded complementary information on metal coordination, resulting structural changes, and consequences for spin probe incorporation. Our results revealed that the presence of metal cations caused distinct changes in the solvation shell of the spin probe. Moreover, we found evidence for complexation occurring between peptide and metal cation[3].

As a second model system we selected L-Carnosine, a dipeptide found in mammalian skeletal muscle. Due to its suggested anti-aging effects, L-Carnosine has recently been popularized as a dietary supplement and cosmetic ingredient[4]. In our ongoing research, we focus on the copper complexes of L-Carnosine, which were found to exhibit free radical scavenging activity[5]. Utilizing CW-EPR and Pulse EPR methods (Hyperfine spectroscopy), we perform an in-depth structural analysis of the complex in solution. By investigating their structure-function relationship, we aim at evaluating their potential as future therapeutic agents.

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Coherent spin manipulation using voltage-controlled oscillators: on path towards single-spin detection

Michal Kern,[1] Mohamed A. Hassan, [1] Maximillian Spieß, [1] Tobias Klotz[1], Zhibin Zhao,[1] Weiyi Zhang,[1] Samuel Wazynski,[1] Klaus Lips, [2] Jens Anders[1,3]

[1] Institute of Smart Sensors, University of Stuttgart, 70569 Stuttgart, Germany; [2] Berlin Joint EPR Laboratory and EPR4Energy, Department Spins in Energy Conversion and Quantum Information Science (ASPIN), Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany; [3] Institute for Microelectronics Stuttgart, IMS CHIPS, 70569 Stuttgart, Germany

michal.kern@iis.uni-stuttgart.de

Inductive detection of electron spins via EPR is nearly universal but fundamentally limited in sensitivity — far from the single-spin level needed for scalable qubit readout. Superconducting resonators have approached this limit [1], but require millikelvin temperatures and are inherently narrowband. We pursue a different route based on voltage-controlled oscillators (VCOs): integrated microwave circuits that generate their own signal and respond to changes in their electromagnetic environment, including the magnetic susceptibility of nearby spins. Unlike passive resonators, VCOs offer broadband frequency tunability, on-chip integration, and compatibility with standard semiconductor processes.

We have demonstrated VCO-based detection of coherent electron [2] and nuclear spin dynamics [3], including spin echoes [4], and extended the approach to 263 GHz using injection-locked oscillator arrays [5]. Sensitivity models predict that single-spin detection becomes accessible around 330 GHz and 2–4 K with inductor diameters of ~10 µm, a regime now reachable with cryo-compatible SiGe BiCMOS and III–V technologies.

In this poster, we present the current state of the platform for coherent spin control and outline the path toward single-spin sensitivity.

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Ferro- and Antiferromagnetic Resonance Studies on Two-Dimensional Quantum Magnets

R. Klingeler

[1] Kirchhoff Institute for Physics, Heidelberg University, Germany

klingeler@kip.uni-heidelberg.de

High-frequency electron spin resonance (HF-ESR) spectroscopy is susceptible to collective spin excitations and hence allows us to explore the low-energy magnon spectra and their magnetic field dependence. We have used HF-ESR to investigate, e.g., the spin structure, domain formation in ferromagnets, magnetic anisotropies, and the evolution of short- and long-range magnetic order in a variety of quasi-2D magnets, including ferromagnets and (quantum) antiferromagnets. Here, we report (1) the quasi-2D Ising antiferromagnet Li_2FeSiO_4 [1], (2) the role of anisotropy for the evolution of long-rang ferromagnetic order in metallic Fe_3GeTe_2 [2] and semiconducting CrI_3 [3], (3) the evolution of magnetic order in a layered triangular antiferromagnet $GdInO_4$ [5], and on the ground state and quantum-criticality in the Kitaev system $Na_2Co_2TeO_6$ [4].

The latter example illustrates the strength of HF-ESR: $Na_2Co_2TeO_6$ is proposed to be proximate to a quantum spin liquid state but a suitable spin model and the nature of its ground states are still under debate. For in-plane magnetic fields, we investigate the quantum critical endpoint. In contrast, for B||c axis, the observation of three distinct spin wave modes in the antiferromagnetic ground state reveals a previously unresolved splitting of the zero-field excitation gap and a soft mode evidencing a field-induced phase transition. Our spin wave calculations based on the extended Heisenberg-Kitaev model exclude the zigzag ground state of the AFM phase. A triple-q spin configuration correctly predicts two spin wave modes but fails to reproduce the softening mode. Our analysis shows that the triple-q ground state model of $Na_2Co_2TeO_6$ is explains several modes but is still incomplete and suggests the relevance of interlayer interactions.

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Direct derivative driving of optically detected magnetic resonance spectra

Tilen Knaflič,[1] Mario Grüneberg,[1] Enrique Sánchez-Ibáñez,[1] Matthijs Ignacy Olivier Vanrooij,[1] Matthäus Hirsch,[1] Claudius Mullen,[1] Jaka Pribošek[1]

[1] Silicon Austria Labs, Villach, Austria

tilen.knaflic@silicon-austria.com

Over the past decade, research on nitrogen-vacancy (NV) centers in diamond has surged, spanning both fundamental studies and applied developments. Their unique spin-dependent optical properties enable optically detected magnetic resonance (ODMR), which has become the central technique for probing NV spin states and the basis of highly sensitive diamond magnetometry. NV-based DC magnetometers have recently achieved pT-level sensitivities, positioning them among the most promising quantum sensing platforms [1,2]. To reach such performance, many DC magnetometry protocols employ frequency modulation (FM) combined with lock-in detection, producing a first-derivative resonance profile. While the resonance zero-crossing, enhanced spectral slope, and lock-in noise rejection collectively improve sensitivity, they also increase the complexity of the measurement hardware. Retaining the sensitivity benefits of FM detection without the associated hardware complexity is highly appealing. In this work, we propose to generate pseudo-derivative response by direct microwave driving through a weighted multitone sweep with weights chosen as convolution filter of smooth first-order derivative kernel. The technique involves two such scans with opposite derivative phases, followed by a simple subtraction to retrieve the pseudo-derivative signal. We analyse the theoretical limitations of this method for both continuous and discrete excitation schemes, discuss the choice of optimal kernels, and experimentally implement the discrete 7-tone case on a commercial diamond sample with a 4.5 ppm NV center concentration. The experimental results show excellent agreement with theory. Finally, we optimize the 7-tone experimental parameters and estimate the resulting DC magnetometry sensitivity.

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Understanding SiC Surface Modification during Si- and C-Cap Annealing through EDMR Studies

Kazumasa Kojima,[1] Oleksii Laguta,[2] Takahito Fukuzawa,[1]
Seiichiro Higashi,[1] Petr Neugebauer,[2] Hiroaki Hanafusa,[1]

[1]Grad. Sch. of Adv. Sci. and Eng., Hiroshima University, Hiroshima, Japan,
[2]CEITEC, Brno University of Technology, Brno, Czech Republic

semicon@hiroshima-u.ac.jp

Conventional metal-silicide-based ohmic contacts for SiC power devices face reliability issues at high temperatures. To overcome this limitation, we proposed silicon-cap annealing (SiCA), which enables low-resistance ohmic contact formation without metal silicides. Defects generated near the SiC surface during annealing are thought to contribute to this behavior, but their identity and role in electrical conduction remain unclear. We have investigated SiCA-treated samples using electrically detected magnetic resonance (EDMR). Although EDMR signals have been observed, the defects responsible for ohmic contact formation have not yet been identified. We are therefore optimizing the sample structures and measurement conditions to improve signal detection. We also examined carbon-cap annealing to distinguish the effect of silicon supplied from the cap from annealing-induced changes in the SiC surface. Good ohmic characteristics were obtained after carbon-cap annealing. This result suggests that changes occurring near the SiC surface during annealing, rather than silicon supply alone, may play an important role in ohmic contact formation. In this presentation, we report our results on Si- and C-cap annealing, together with the EDMR findings obtained to date. We also discuss future EDMR-based evaluation methods for clarifying the relationship between annealing-induced defects, electrical conduction, and ohmic contact formation.

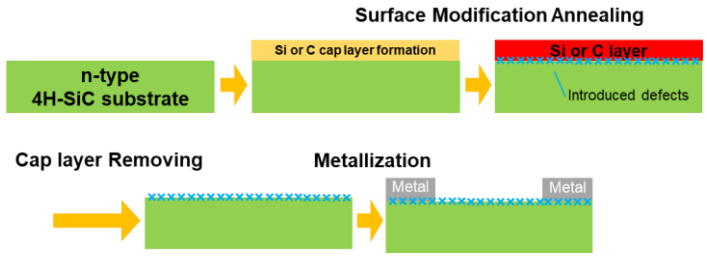

Figure 1: Schematic illustration of the Si- and C-cap annealing processes for silicide-free ohmic contact formation on n-type 4H-SiC.

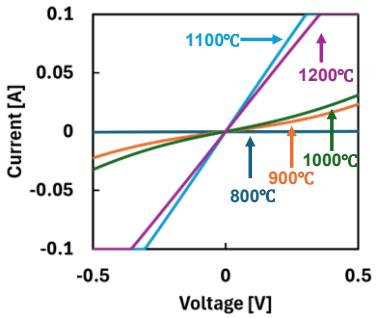

Figure 2: I-V characteristics at different C-cap annealing temperatures.

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Stimuli-Responsive Binitroxide Hydrazone Molecular Switches

Lucie Kotásková,[1] Vinicius Santana,[1] Oleksii Laguta,[1] Petr Neugebauer[1]

[1] Central European Institute of Technology, Brno University of Technology, Purkyňova 656/123, 61200 Brno, Czech Republic

Lucie.Kotaskova1@ceitec.vutbr.cz

Stable nitroxide radicals are versatile paramagnetic building blocks whose unique sensitivity to the local environment makes them powerful tools for introducing functional spin centers into responsive molecular systems.[1] However, combining these radicals with hydrazone-based molecular switches remains largely unexplored despite the attractive properties of both motifs. Here we introduce a new class of binitroxide hydrazone switches integrating two TEMPOL radicals into a single stimuli-responsive framework. The reversible isomerization of the hydrazone core enables controlled modulation of the inter-radical distance and molecular geometry.

Two model systems featuring either a pyridine or phenyl rotor were prepared using a Mitsunobu strategy. The switching studies highlight a deliberate structure-property tuning: pyridine-based switch operates as a dual photo- and pH-responsive switch, while the phenyl derivative was rationally designed to enhance photochemical performance by eliminating intramolecular hydrogen bonding, resulting in highly efficient, nearly quantitative photoisomerization. While ^{1}H NMR confirms the isomerization into the less stable state, EPR spectroscopy verifies the fully preserved paramagnetism with negligible spin-spin interactions due to the large inter-radical distance.

These binitroxide switches establish a versatile platform for stimuli-controlled modulation of magnetic interactions, opening new opportunities in supramolecular assemblies, spin probes, and adaptive polarizing agents for dynamic nuclear polarization.

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Surfactant-Free EPR Probing of Linoleic Acid Peroxidation: Optimizing Sensitivity and Concentration Thresholds in Acetonitrile

Jakub Kovář,[1,2] Pedro H. O. Santiago,[1] Vinicius T. Santana[1]

[1] Central European Institute of Technology (CEITEC), Brno University of Technology, Brno, Czech Republic.

[2] Department of Biomedical Engineering, Faculty of Electrical Engineering and Communication, Brno University of Technology, Brno, Czech Republic.

247258@vut.cz

Lipid peroxidation is a destructive free-radical chain reaction initiated when reactive oxygen species (ROS) abstract allylic hydrogen atoms from polyunsaturated fatty acids (PUFAs), such as linoleic acid, causing the degradation of cell membrane. Pathologically, this transition metal-catalyzed oxidative damage severely compromises cellular membrane integrity and generates toxic secondary lipid electrophiles. Consequently, uncontrolled lipid peroxidation is a primary driver in the pathogenesis of numerous conditions, including neurodegenerative diseases, atherosclerosis, and cellular aging.[1] Conventional *in vitro* studies of lipid peroxidation rely on aqueous surfactant emulsions or micellar systems to solubilize polyunsaturated fatty acids. However, surfactants frequently introduce kinetic artifacts, alter local micro-viscosity, and can act as unintended radical scavengers.[2] This work proposes an improved, surfactant-free methodology for monitoring metal-catalysed lipid peroxidation in a homogeneous organic medium. Using a $CuCl_2/H_2O_2$ initiating system in acetonitrile with DMPO as a spin trap, we first characterized the baseline hydroxyl radical generation and address spectroscopic challenges, including Cu^{2+}-induced paramagnetic dipole relaxation and line broadening.[3] Building on this optimized baseline, the primary objective of this study is to determine the lowest threshold concentration of linoleic acid required to generate interpretable, statistically meaningful EPR spin-adduct spectra. By eliminating surfactant-induced compartmentalization and establishing sensitivity limits, this surfactant-free approach can provide a cleaner and highly reproducible framework for evaluating true radical kinetics during the initiation and propagation of lipid peroxidation.

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Engineering iLOV for Enhanced Spin Polarization: Linking Protein Structure, FMN Photophysics, and EPR

Sebastian Krebs,[1] Luca Gerhards,[2] Matthias Elgeti[1,3]

[1] Institute for Drug Discovery, University of Leipzig Medical School; [2] Department of Physics, Carl von Ossietzky University; [3] Institute of Medical Physics and Biophysics, University of Leipzig Medical School

Sebastian.Krebs@medizin.uni-leipzig.de

Light-oxygen-voltage-sensing (LOV) domains are small, genetically encoded flavin mononucleotide (FMN) binding photoreceptors. Following blue-light excitation, FMN undergoes competing radiative and non-radiative processes governed by the electrostatics, hydrogen-bonding network, and rigidity of the FMN-binding pocket.[1] In native LOV domains, intersystem crossing populates the triplet state, which predominantly initiates formation of a covalent FMN-cysteine adduct. Substitution of the conserved cysteine prevents this reaction and redirects triplet-state photochemistry towards electron transfer, radical-pair formation, and photoreduced FMN species detectable by EPR.[2] Cysteine-free variants also generate strong photochemically induced dynamic nuclear polarization, demonstrating light-induced spin order in LOV proteins.[3] However, the structural factors controlling intersystem crossing, electron transfer, and polarization efficiency remain insufficiently understood.

To investigate this structure-function relationship, we use iLOV, an engineered fluorescent derivative of the LOV2 domain of Arabidopsis thaliana phototropin 2.[4] iLOV mutations are reverted towards the wild-type AtPhot2-LOV2 sequence to probe the effects of pocket rigidity and electrostatics. In parallel, candidate Trp and Tyr electron donors are individually replaced with Phe or Ser to examine their contributions to FMN binding and electron transfer.

Ten mutants were expressed, purified, and characterized by UV/Vis and fluorescence spectroscopy to assess FMN occupancy and fluorescence properties. Light-induced CW-EPR was subsequently used to characterize semiquinone formation. Time-resolved EPR measurements on selected mutants will characterize triplet formation and electron-spin polarization. Molecular-dynamics simulations and quantum-mechanical calculations will relate the spectroscopic observations to structural changes, electrostatics, excited-state energetics, and electron-transfer pathways. This integrated approach aims to establish design principles for spin-polarizing LOV proteins and light-driven hyperpolarization sources.

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Multiple quantum ^{19}F electron-nuclear double resonance (ENDOR) for distance measurements with multifluorinated spin probes

Sergei Kuzin,[1] Lucca Sielaff,[1,2] Marina Bennati[1,2]

[1] MPI for Multidisciplinary Sciences, Göttingen, Germany; [2] University of Göttingen, Göttingen, Germany;

sergei.kuzin@mpinat.mpg.de

Mims electron-nuclear double resonance (ENDOR) spectroscopy with ^{19}F spin labels is emerging as a powerful tool to access molecular distances in the 5-20 Å range in biomolecules. The recently developed time-domain (TD) version of this experiment allows manipulation of nuclear spin coherences, similar to NMR, and thereby increases the distance resolution.[1] Nevertheless, Mims ENDOR sensitivity strongly decays with the inter-spin distance *r*, and measurements of longer distances benefit from labels with multiple ^{19}F nuclei, such as CF_3 probes.

We demonstrate that TD Mims ENDOR with two or three ^{19}F nuclei reveals multiple-quantum effects as well as homonuclear dipolar couplings.[2] These effects allow for deeper characterization of molecular geometry in multifluorinated systems. For example, excitation of double-quantum nuclear coherence enables correlation of electron-^{19}F distances in a molecule – information not readily accessible by standard spectroscopic techniques. We developed a general theoretical framework for TD Mims ENDOR with multiple like nuclei (i.e., ^{19}F), facilitating analysis of spin evolution and the controlled experimental generation of single- and multiple-quantum nuclear coherences. The theoretical model was validated with several rationally designed nitroxide radicals bearing two and three ^{19}F labels (Figure 1). The agreement with theory was demonstrated in a broad range of experimental parameters.

Our results directly report not only on electron-nuclear distances but also on measurements of inter-nuclear distances and distance distributions between like nuclei. Overall, TD ENDOR potentially offers a new toolbox for (bio)molecular structure investigations.

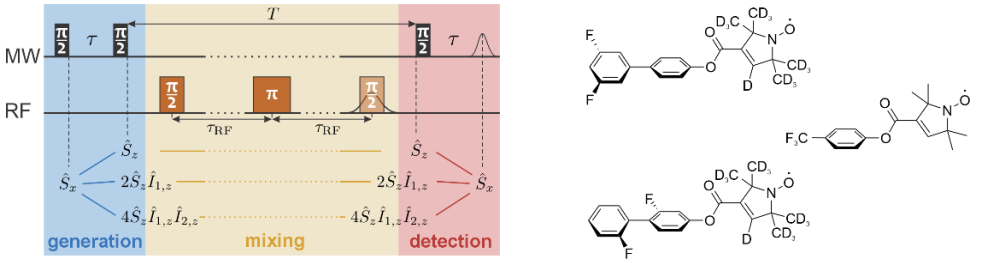

Figure 1: Time-domain ENDOR experiment (left) and studied compounds (right).

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ESR Probing of Carboxylate- and Crystallization-Controlled Nuclearity Switching in Cu(II) Complexes

David Kučera-Čavara,[1] Enis Šuta,[2] Nevzeta Ljubijankić,[2] Adnan Zahirović,[2] Aleksandar Višnjevac,[1] Dijana Žilić[1]

[1] Division of Physical Chemistry, Ruđer Bošković Institute, Zagreb, Croatia;
[2] Department of Chemistry, Faculty of Science, University of Sarajevo, Sarajevo, Bosnia and Herzegovina

dakuceracavara@irb.hr

A series of Cu(II) carboxylate complexes derived from a quinoline-based mono-imine ligand (HL) was synthesized to investigate structural switching governed by carboxylate identity and crystallization conditions. The objective of this study is to utilize electron spin resonance (ESR) spectroscopy to differentiate between the distinct structural forms, confirm the presence of monomeric or dimeric complexes, and evaluate their structural stability in solution. To investigate the local electronic environment of different complexes, the continuous-wave (CW) ESR spectroscopy was employed at room and liquid nitrogen temperatures. For all investigated complexes, spin state S = 1/2 was assigned to the Cu(II) ions [1]. Simulations of the experimental spectra were performed using the EasySpin software [2]. As shown in Figure 1, the transformation of the amorphous precursor $(1)^{am}$ into the crystalline complexes $(3b)^{crys}$ and $(4)^{crys}$ results in a clear distinction in their ESR spectra. These findings highlight the sensitivity of ESR spectroscopy to subtle structural changes in copper(II) carboxylates.

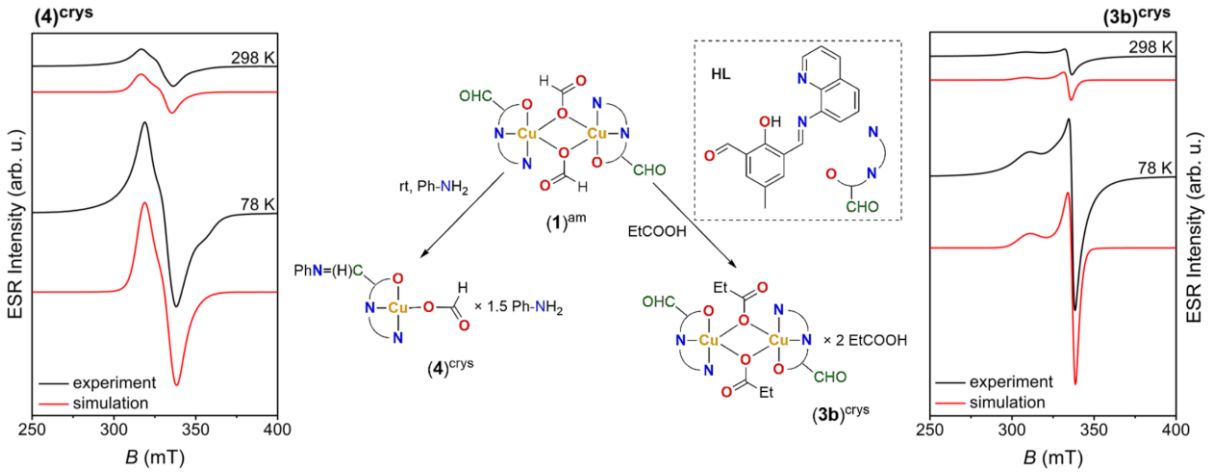

Figure 1: Solid-state experimental and simulated ESR spectra of the complexes $(3b)^{crys}$ and $(4)^{crys}$.

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Electrical Control and HFEPR Investigation of Single-Molecule Magnets on Two-Dimensional Materials

Sujan Maity,[1] Jorge Navarro-Giraldo,[1,2] Petr Neugebauer[1]

[1] Central European Institute of Technology – Brno University of Technology, CEITEC BUT, Purkyňova 656/123, 61200 Brno, Czech Republic

[2] Institute of Molecular Science-ICMOL, University of Valencia, Valencia, Spain

e-mail address presenting author: maity@vutbr.cz

Single-Molecule Magnets (SMMs) are promising building blocks for molecular spintronics and quantum technologies because of their magnetic bistability, large magnetic anisotropy, and long spin coherence times. Integrating SMMs with two-dimensional (2D) materials offers new opportunities for electrical control and readout of molecular spin states while preserving their intrinsic magnetic properties. In this work, we investigate hybrid heterostructures consisting of cobalt-based SMMs deposited on graphene, transition metal dichalcogenides (WS_2 and MoS_2), and topological insulators (Bi_2Se_3 and Bi_2Te_3).

The study focuses on optimizing sub-monolayer deposition of SMMs [1] and characterizing their magnetic properties using high-frequency electron paramagnetic resonance (HFEPR) spectroscopy [2] with an integrated Fabry–Pérot resonator to achieve enhanced sensitivity for ultrathin molecular films. Electronic transport, magnetotransport, and field-effect transistor measurements will be performed to examine charge transfer at the molecule–2D material interface [1] and to investigate electrostatic gate-controlled modulation of molecular spin states. The influence of substrate spin–orbit coupling on spin transport and molecular magnetism will also be explored, together with microwave-driven manipulation of molecular spin states.

This work combines advanced HFEPR spectroscopy with transport measurements to establish scalable approaches for probing and controlling molecular magnetism in hybrid SMM–2D material systems. The results are expected to provide new insights into molecule–substrate interactions and support the development of electrically addressable molecular spintronic and quantum devices.

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DFT study of carbon- and silicon-based nanomaterials: electronic structure, spin state preference, and hydrogen storage performance

Michal Malček, Ondrej Tkáč

Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic

Corresponding author: michal.malcek@stuba.sk

Since the isolation of graphene in 2004, 2D materials attracted a considerable attention due to their extraordinary properties [1]. A couple of years later, 2D silicon sheet, named silicene, was synthesized by chemical exfoliation of $CaSi_2$ [2]. In the presented study, DFT calculations, QTAIM analysis and ab initio molecular dynamics are employed to investigate the various graphene- and silicene-based nanomaterials modified with transition metal atoms. In these systems, the transition metal atoms can serve as active sites, for example for various types of interaction with H2 molecules (Kubas interactions, H2 dissociation, physisorption). Our studies suggest that there are several important factors affecting the hydrogen binding performance of these systems, such as spin state [3], oxidation state [4], or choice of the metal atom [5].

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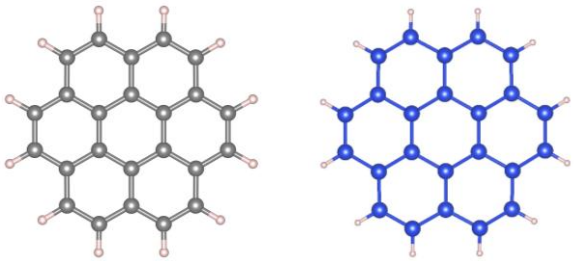

Figure 1: Structure of coronene (left) and its silicon analog (right).

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Indirect EPR Strategies for Investigating Reactive Species in Functional Materials: Pathways and The Importance of Spin-Trap Purity

Miriama Malček Šimunková,[1, 2] Michal Zalibera,[1] Vlasta Brezová,[1] Petr Neugebauer[2]

[1] Department of Physical Chemistry,Institute of Physical Chemistry and Chemical Physics,Faculty of Chemical and Food Technology,Slovak University of Technology, Radlinského 9, 812 37 Bratislava;
[2] European Institute of Technology – Brno University of Technology, CEITEC BUT, Purkyňova 656/123, 61200 Brno, Czech Republic
miriama.simunkova@stuba.sk

Reactive oxygen species (ROS) are key intermediates in advanced oxidation processes (AOPs) used for various applications. Due to their short lifetimes, their direct detection by conventional cw-EPR is often challenging. Indirect EPR techniques, particularly spin trapping, are therefore widely used to identify ROS in activation of various materials. [1] The spin trap 5,5-dimethyl-1-pyrroline *N*-oxide (DMPO) reacts with transient radicals to form longer-lived paramagnetic adducts detectable by EPR. However, interpretation of spin adducts signal requires caution, as it may arise not only from hydroxyl radical trapping but also from alternative pathways e.g. inverted spin trapping and the Forrester–Hepburn mechanism (Figure 1). [2] Accurate ROS identification further depends on spin-trap purity. Oxidative degradation of DMPO during storage produces paramagnetic impurities that can interfere with EPR measurements. To overcome this limitation, we developed a modified short-path molecular distillation that provides highly purified DMPO, enabling more reliable detection and quantification of ROS and other generated radicals.

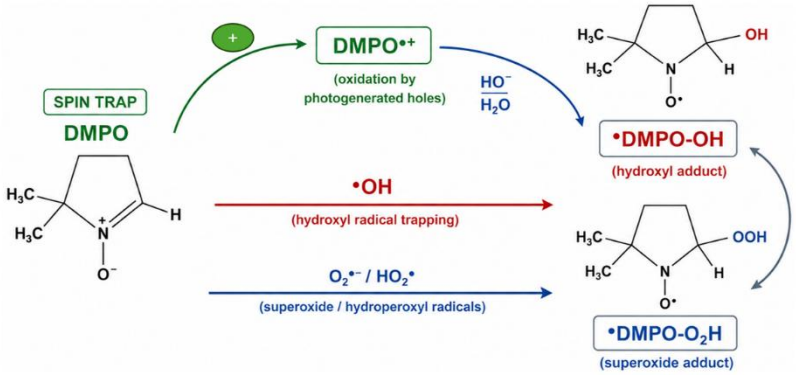

Figure 1: The reaction pathways in DMPO spin trapping

Acknowledgement: This study was supported by APVV project VV-MVP-24-0039 and APVV-24-0460.

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Chirality-induced spin selectivity in single crystals of Photosystem I

Gianluca Marcozzi,[1] Naitik A. Panjwani,[1] Alessandro Chiesa,[2] Stefano Carretta,[2] Robert Bittl[1]

[1] Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195, Berlin, Germany.
[2] Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, I-43124 Parma, Italy.

g.marcozzi@fu-berlin.de

Chirality-induced spin selectivity (CISS) is the phenomenon by which spin polarization is observed upon charge transfer through a chiral medium. Given its reported efficiency at room temperature various application in quantum information and spintronics have been proposed, as well as interpretations about its fundamental role in biology.[1] Nevertheless, a comprehensive understanding of CISS is still missing. Recently, CISS has been observed via transient electron paramagnetic resonance (trEPR) in donor-acceptor systems linked by a chiral bridge (D-χ-A).[2] In these experiments, spectroscopic differences in the trEPR between the D-χ-A systems and their counterparts with an achiral bridge (D-B-A) have been attributed to CISS. The sample used in these investigations are D-χ/B-A frozen in liquid crystals or isotropic solutions, therefore no unidirectional order was present, which would have broken the 180° rotation invariance and provided an indisputable proof of CISS. Here we present the investigation via trEPR of a well characterized biological sample, namely Photosystem I (PSI).[3] Single crystals of PSI present several interesting properties related to CISS: i) Carmeli et al.[4] reported a temperature dependent spin polarization due to CISS in PSI via contact voltage measurements on a capacitance device; ii) the trimeric PSI *of Synechococcus elongatus* crystalizes in the $P6_3$ space group with unidirectional order of all complexes[5]; iii) due to the temperature dependence of CISS, measurements on a single sample would show absence or presence of CISS as a function of the chosen experimental temperature, eliminating the need of any reference sample.

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EPR spin trapping approaches for monitoring radical processes in food systems under non-thermal processing conditions

Franka Markić,[1] Senada Muratović,[1] Nadica Maltar-Strmečki[1]

[1]Ruđer Bošković Institute, Laboratory for Electron Spin Spectroscopy, Division of Physical Chemistry, Bijenička c. 54, 10 000 Zagreb, Croatia

fmarkic@irb.hr

In food science, spin-trapping provides insight into radical formation during processing and storage, particularly under non-thermal conditions. Understanding radical behaviour is essential for assessing food quality, safety, and stability, as conventional techniques often cannot directly detect transient radical species[1].

In this study, EPR spin trapping combined with EPR spectroscopy was used to detect and quantify free radical formation in food systems under non-thermal processing using BMPO, CMH, and DIPPMPO spin traps. Ultrasound-treated aqueous systems and tomato juice were used as simple and complex matrices to evaluate the effect of ultrasound amplitude (30–90%) and treatment time (1–5 min) on radical generation.

The results demonstrate that radical detectability in food systems is strongly dependent on ultrasound processing conditions and matrix composition. BMPO enabled direct detection of ultrasound-induced radicals in aqueous systems, while no detectable signals were observed in tomato juice, indicating a strong matrix effect that limits direct radical trapping in complex food systems. In tomato juice, CMH showed increased signal intensity with sonication, suggesting enhanced radical formation within a matrix rich in naturally occurring bioactive compounds. In contrast, DIPPMPO required post-treatment activation via a Fenton reaction to enable radical detection, indicating the presence of transient radical species with limited stability.

In conclusion, this study confirms that EPR spin trapping is a highly sensitive and reliable analytical method for investigating redox processes induced by non-thermal processing, but further optimization for each technique is needed. The findings indicate that radical formation is strongly dependent on processing parameters, food matrix composition, and the choice of an appropriate spin-trap. Such an analytical approach represents a step towards more sensitive and reliable monitoring of food quality and safety in future food research and processing technologies. This may further support the development of optimized processing strategies that minimize undesirable oxidative changes in foods.

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Ferrocenium encapsulated in α-cyclodextrin: controlling magnetic relaxation mechanisms

Jesús I. Martínez,[1] Adriana Silvestre-Llora,[2] Fernando Luis,[1] Silvia Gómez-Coca,[2] Eliseo Ruiz[2]

[1] Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC and Universidad de Zaragoza, Plaza San Francisco s/n, 50009 Zaragoza, Spain; [2] Departament de Química Inorgànica i Orgànica and Institut de Recerca de Química Teòrica i Computacional, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain

e-mail address: jimartin@unizar.es

Ferrocenium is a paramagnetic center consisting of an Fe(III) ion sandwiched between two cyclopentadienyl rings. Although its state can be treated using the strong-field approximation, the ground state is not the one predicted by the molecular symmetry, as interelectronic repulsion leads to *non-Aufbau* occupation of the orbitals. Furthermore, the iron orbitals involved exhibit strong mixing with the π orbitals of the rings. Ferrocenium and its derivatives have been characterized by EPR since the 1950s [1,2]. In recent years, they have once again attracted interest in the field of nanomagnetism, as candidates for SMMs or electronic spin qubits [3,4]. In this presentation, we will describe a comprehensive study, using CW- and pulse EPR, magnetic characterization, and calculations, of ferrocenium encapsulated in the organic molecule α-cyclodextrin. Encapsulation allows for the creation of isolated ferrocenium entities, reducing relaxation pathways. Furthermore, solid solutions of the paramagnetic entities into encapsulated cobaltocenium (which is diamagnetic) can be grown. This allows controlling the distribution of Fe-Fe distances within the structure. In this way, the contributions of the different relaxation mechanisms to the spin-spin and spin-lattice times in this system were determined, which can be used to optimize the properties of ferrocenium as a material for nanomagnetism.

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Spin-Probe EPR Study of Decalin and Perfluorodecalin Liquids

Dalibor Merunka,[1] Miroslava Lukešová[1]

[1] Ruđer Bošković Institute, Zagreb, Croatia

merunka@irb.hr

We used ^{14}N- and ^{15}N-labeled perdeuterated TEMPONE radicals as spin probes in an EPR study of the molecular liquids *cis*-decalin, *trans*-decalin, and *cis*-perfluorodecalin.[1] We measured EPR spectra of the radicals in deoxygenated liquids while cooling from their equilibrium liquid state above the melting point T_m to their supercooled state below T_m.

By fitting the EPR spectra of the radicals to theoretical spectral functions, we found that the best-fit EPR parameters exhibit an anomalous temperature dependence in both decalins, but not in *cis*-perfluorodecalin. One example is the temperature dependence of the nitrogen hyperfine coupling constant A of the radicals, which shows an anomalous maximum in the decalins and normal behavior in *cis*-perfluorodecalin (Figure 1).

The explanation for this behavior is that *cis*-perfluorodecalin behaves as a normal homogeneous liquid, while the decalins transform from homogeneous to heterogeneous liquids upon cooling below about 300–320 K.[1] The heterogeneous liquid structure of decalins is a rather unique property among molecular liquids, and its origin and character deserve further investigation. This work is supported by the Croatian Science Foundation (Project HRZZ-IP-2022-10-9292).

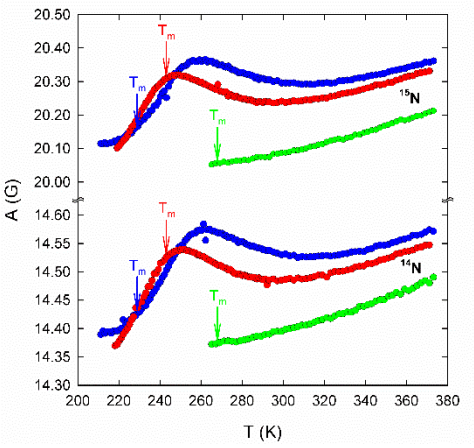

Figure 1: Nitrogen hyperfine coupling constants of ^{14}N- and ^{15}N-labeled perdeuterated TEMPONE in molecular liquids *cis*-decalin (blue), *trans*-decalin (red), and *cis*-perfluorodecalin (green).

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Microwave-induced transitions between weak localization and weak antilocalization in graphene

Jorge Navarro-Giraldo[1*], Vinicius T. Santana[1], Oleksii Laguta[1], Dominik Bloos[2], Anastasia Bauernfeind[3], Marc Scheffler[3], Valentyn Laguta[4], D. Kurt Gaskill[5], and Petr Neugebauer[1]

[1]Central European Institute of Technology – Brno University of Technology, CEITEC BUT, Brno, Czech Republic; [2]Institute of Physical Chemistry, Universität Stuttgart, Stuttgart, Germany; [3]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany; [4]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic; [5]Institute for Research in Electronics and Applied Physics, University of Maryland, Maryland, USA.

[*]*Currently at Institute of Molecular Science* –ICMOL, *University of Valencia, Spain* jorge.a.navarro@uv.es

Weak localization (WL) and weak antilocalization (WAL) are quantum effects that emerge from the phase-coherent electronic transport in a 2D system. They typically appear at low temperatures and are detected by DC magneto-transport experiments. In this work,[1] using setups commonly employed for electron paramagnetic resonance, we characterize the WL in monolayer graphene by contactless microwave spectroscopy. We demonstrate that when the microwave frequency is smaller than the electron decoherence rate, the spectroscopic measurements agree well with DC transport experiments. At frequencies much higher than the decoherence rate ($\omega/2\pi$ = 90–350 GHz), the microwaves induce transitions between WL and WAL previously not observed in the literature. This study unravels novel phenomena emerging from electron interaction with sub-THz radiation, and highlights microwave spectroscopy as a valuable tool for the transport characterization of solid-state systems.

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Nickel Complexes with Amidrazone Schiff Base Ligands

Ing. Lenka Novotná,[1] Ing. Michal Zalibera, PhD.,[1]

[1] Department of Physical Chemistry, FCHPT STU Bratislava

lenka.novotna@stuba.sk

Amidrazone Schiff bases represent a promising class of ligands due to their tunable electronic properties and redox non-innocence. In contrast to previously reported analogues, their exclusively nitrogen-based coordination avoids unwanted side reactions, making them attractive candidates for catalytic applications — for example, the selective oxidation of cyclohexane, a key yet still poorly selective step in nylon production. [1,2]
In this work, mono- and dinuclear nickel complexes bearing amidrazone Schiff base ligands were characterized. Their redox properties were investigated by cyclic voltammetry, UV-Vis-NIR spectroelectrochemistry, and EPR spectroscopy, complemented by chemical reduction with cobaltocene. Complexes 6 and 7 exhibited reversible, multi-step (two-electron) transitions. Semi-integration of the CV signal confirmed the two-electron character of the first reduction of complex 7. EPR spectroscopy revealed a singlet ground state with a thermally populated triplet for complex 6, transitioning to a doublet upon the first reduction, while complex 7 is EPR silent in its neutral state and shows a ligand-centered radical with hyperfine coupling to two equivalent ^{14}N nuclei upon reduction, confirming spin delocalization over the ligand.
These findings indicate that complexes 6 and 7, owing to their reversible, stepwise electron transfer and ligand-mediated redox activity, are promising candidates for the further development of catalysts.

This work was supported by VEGA under Contract No. 1/0392/24 and by APVV under Contract No. APVV-23-0195.

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Design and Optimization of Carousel holder for EPR Spectroscopy

Pelikán Petr,[1,2] Šťastný Přemysl,[1] Laguta Oleksii[1]

Neugebauer Petr[1]

[1] Central European Institute of Technology (CEITEC), Brno, Czech Republic

[2] Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic

267572@vutbr.cz

Quantitative analysis in high-frequency electron spin resonance (HF-ESR) spectroscopy is frequently constrained by the time-intensive nature of sample exchange, which necessitates repeated thermal cycling and vacuum disruption. To address this methodological limitation and improve the efficiency of routine measurements, we report the design and implementation of a novel vacuum carousel accommodating six samples. The primary objective of this hardware development is to ensure reliable sample positioning and consistent microwave coupling while significantly reducing the time required for sample exchange.

The carousel allows for the in situ automated switching of six samples directly inside the cryostat, effectively eliminating the need for recurrent cooling and heating procedures. To optimize the thermal performance, the structural geometry was designed specifically for ceramic 3D printing using aluminum oxide (Al2O3). This material exhibits high thermal conductivity, facilitating rapid thermal equilibration. Alongside the six sample positions, the system integrates a temperature sensor and a heating resistor mounted on a highly conductive mirror. This configuration, in synergy with the Al2O3 structure, yields an overall temperature stability of 0.05 K. Furthermore, the system integrates easily assembled Helmholtz coils for localized magnetic field manipulation and rapid field modulation. By minimizing operational downtime, this robust hardware design improves user comfort and facilitates cost-effective, high-throughput experiments in high-field EPR spectroscopy.

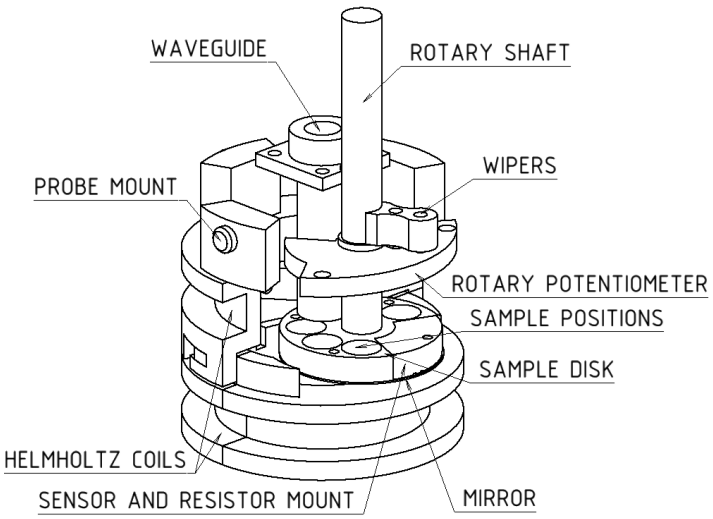

Fig. 1 Annotated 3D carousel schematic.

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EPR insight into ROS generation pathways over redox and non-redox materials: interfacial electroprotic reactions of H_2O_2

Piotr Pietrzyk,[1] Kamila Sobańska[1]

[1] Faculty of Chemistry, Jagiellonian University, ul. Gronostajowa 2, 30-387 Kraków, Poland

piotr.pietrzyk@uj.edu.pl

Research on the role of transition-metal oxides as catalysts for H_2O_2 decomposition and radical formation (the so-called peroxidase-like activity) has recently emerged as a critical area of inquiry due to its broad applications in environmental remediation, chemical synthesis, and energy conversion. The practical significance lies in the ability of these materials to generate ROS, such as hydroxyl ($^{\bullet}OH$) and superoxide ($O_2^{\bullet-}$) radicals, which are potent oxidants for degrading organic pollutants and facilitating oxidation reactions. In this contribution, we show comprehensive spectroscopic analysis of the interaction between aqueous H_2O_2 and two types of oxide materials: typical Fenton-type oxides and amorphous, non-redox materials. We aimed to analyse and detect ROS formed during this interaction, focusing on the various chemical parameters of H_2O_2 decomposition.

In particular, non-redox, amorphous oxides of zirconium, hafnium, niobium, and tantalum are found active in ROS formation via H_2O_2 decomposition. Various intermediates such as $O_2^{-\bullet}$ and $^{\bullet}OH$ radicals, O_2^{2-} species were identified. The radicals were generated simultaneously, with peak concentrations near the catalysts' isoelectric points (IEPs). In this pH region, the amorphous oxides exhibited peroxidase-like activity. Above IEP, a substantial release of O_2 due to catalase-like activity and generation of $^1O_2$ was observed. The results were accounted for by an electroprotic mechanism of H_2O_2 activation, in which the interplay between the simultaneous generation of hydroxyl and superoxide radicals and the surface stabilization of selected ROS was decisive.[1] Based on this mechanism, the environmental methylene blue (MB) degradation process was accounted for. The observed activity decreased in the order ZrO_2 > Nb_2O_5 ~ HfO_2 >> Ta_2O_5, and correlated with the overall ROS level. Both types of activity in wet peroxidation contributed to the observed MB degradation: peroxidase-type via electroprotic mechanism resulting in $^{\bullet}OH$, complemented with catalase-type activity resulting in $^1O_2$.

Acknowledgement: This work was financially supported by the National Science Center, Poland (NCN), grant OPUS27 2024/53/B/ST4/03929.

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Towards X-band EPR cryoprobe based on a bimodal cavity

Ignas Pocius,[1] Vidmantas Kalendra,[1] Gediminas Usevičius, [1] Jūras Banys,[1] Mantas Šimėnas[1]

[1] Vilnius University, Faculty of Physics, Institute of Applied Electrodynamics and Telecommunications, Lithuania

ignas.pocius@ff.vu.lt

We present a design of a microwave cryoprobe featuring a bimodal resonant cavity with two orthogonal X-band modes. In bimodal resonant cavities one of the modes excites the spins in the sample, while the other mode is used to read out the EPR signal (see Figure 1). A cryoprobe with such a resonator geometry prevents the resonator ringing effect [1-3] and can be used to suppress thermal noise greatly enhancing EPR sensitivity. A bimodal X-band microwave resonator based on the design proposed in Ref. [1] with appropriate modifications for our use-case was manufactured and its suitability for our proposed cryoprobe was experimentally evaluated.

Figure 1: A basic loop-gap resonator in single mode and bimodal geometries.

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Reactivity of Cu-based compounds in Fenton-type degradation of model water toxicants: EPR study using spin traps and ROS quenchers

Piotr Pietrzyk,[1] Wiktor Czerwonka,[1,2] Kamila Sobańska[1]

[1] Faculty of Chemistry, Jagiellonian University, ul. Gronostajowa 2, 30-387 Kraków, Poland, [2] Doctoral School of Exact and Natural Sciences, Jagiellonian University, ul. Prof. St. Łojasiewicza 11, 30-348 Kraków, Poland

piotr.pietrzyk@uj.edu.pl

Advanced oxidation processes (AOPs) have emerged as one of the most promising technologies for the removal of persistent pollutants and the remediation of water. Their exceptional effectiveness arises from the in situ generation of highly reactive oxygen species (ROS), including hydroxyl, sulfate, and superoxide radicals, as well as singlet oxygen, which are capable of rapidly oxidizing a broad spectrum of toxicants. As a result, EPR spectroscopy become naturally one of the characterization techniques of the prime choice.[1] In recent years, the integration of AOPs with heterogeneous catalysis has significantly expanded their potential, enabling higher reaction efficiency. The development of catalytic materials, combined with a deeper understanding of reaction mechanisms and ROS generation pathways, has opened new opportunities for designing sustainable technologies. Such a mechanistic insight can be obtained using an indirect detection of elusive ROS by spin-trapping technique combined with spectroscopic and catalytic measurements in the presence of selective ROS quenchers.[2] As scavengers react more rapidly with ROS, they slow down the pollutant's degradation after a specified time. Furthermore, using selective scavengers enables the contribution of specific ROS to pollutant degradation to be determined. However, it is important to note that certain redox catalysts are not susceptible to scavenging, and in some cases, scavengers can actually accelerate the reaction.

In this study, a series of Cu-based materials obtained via solvothermal and precipitation routes was tested as Fenton-like catalysts using H_2O_2 as a benign oxidant. This examination was conducted using the EPR spectroscopy. The study endeavour to assess the evolution of ROS speciation in relation to catalyst composition and surface active sites. Such studies are anticipated to enhance the precision of structure-activity-selectivity relationships, and as a result to optimisation of catalysts under authentic water treatment conditions.

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Ni(II), Cu(II) and Zn(II) complexes with a redox-noninnocent Schiff bases bearing a disiloxane unit – EPR and UV-vis-NIR spectroelectrochemistry

Peter Rapta[1]

[1] Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, SK-81237 Bratislava, Slovakia.

peter.rapta@stuba.sk

The noninnocent behaviour of Ni(II), Cu(II) and Zn(II) complexes with a redox-noninnocent Schiff bases bearing a disiloxane unit was investigated by electrochemical and EPR/UV-Vis-NIR spectroelectrochemical techniques. Recently, we reported that 2-hydroxybenzaldehyde and related derivatives react with 1,3-bis(3-aminopropyl)tetramethyldisiloxane in the presence of Ni(II), Cu(II) or Zn(II) with the formation of tetrahedrally distorted square-planar metal(II) complexes of tetradentate Schiff bases with a trans-arrangement of N_2O_2 donor atoms [1-3]. Two consecutive one-electron reversible electrochemical oxidations are accompanied by a decrease of the absorptions in the UV region of the optical spectrum and simultaneous appearance and further development of new optical bands in Vis-NIR region due to formation of phenoxyl mono- and di-radicals, respectively. The spectroelectrochemical experiment performed for nickel(II) complex coupled with EPR measurements at 100 K confirmed the formation of $[Ni(II/III)L]^+$ species with strong noninnocent character exhibiting a rhombic EPR signal with a large g-tensor anisotropy. The DFT calculations have shown that the one-electron oxidised Cu(II) complex should exist in the triplet ground state with one unpaired electron located on d_{x2-y2} orbital of Cu(II) (d^9, S = ½) and another unpaired electron located on the MO including p_z orbitals of oxygen and carbon atoms of the phenoxyl moiety. Following the theoretical analysis of the localized orbitals it can be concluded that Ni is the redox active site in the first step of oxidation, leading to a Ni(II)/Ni(III) intermediate. In the second oxidation step, the ligand becomes oxidized, and the formal electronic d^8 configuration, Ni(II), is restored. In the case of Cu(II) complexes the ligand is initially oxidized, and copper remains in the d^9 configuration during both oxidation steps.

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Tunable Electron Quantum Optics in Graphene

Mohamed Amine Rhanbouri,[1] Wojciech Julian Pasek,[1] Abdelouahed El Fatimy[1]

[1] College of Physical Sciences and Engineering, Mohammed VI Polytechnic University, Ben Guerir, 43150, Morocco

MohamedAmine.RHANBOURI@um6p.ma

Graphene combines long phase-coherence lengths with a valley degree of freedom absent in conventional two-dimensional electron gases, making it an attractive platform for electron quantum optics. We propose a graphene slit junction as a compact geometry combining valley-dependent beam formation, coherent interference, and symmetry-controlled spin filtering in a single device. Using tight-binding calculations and the nonequilibrium Green's function formalism, we show that trigonal warping generates two highly directional valley-polarized electron beams emitted from the slit and separated by 60°[1]. Reflected by the device edges, the beams recombine at the drain electrode, giving rise to Aharonov–Bohm interference controlled by magnetic flux and electrostatic gating; the oscillations vanish when the energy is detuned from the trigonal-warping regime, confirming their valley origin. Within a mean-field Hubbard description, the zigzag edges created by the slit host magnetic moments: the symmetric junction has an antiferromagnetic, spin-unpolarized ground state, while breaking the left/right symmetry, via edge defects or electrostatically defined p–n junctions, induces spin-polarized transmission[2]. The mechanism relies only on the Fermi-surface anisotropy and remains relevant in bilayer graphene, where trigonal warping is accessible at much lower, gate-tunable energies[3,4].

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ESR Measurements with Superconducting Coplanar Resonators

Florentine Scharwaechter[1], Nicolai Schröter[2], Martin Dressel[1], Lorenzo Tesi [2], Marc Scheffler[1]

[1]1. Physikalisches Institut, Universität Stuttgart, D-70569 Stuttgart, Germany; [2]Institut für Physikalische Chemie, Universität Stuttgart, D-70569 Stuttgart, Germany

florentine.scharwaechter@pi1.uni-stuttgart.de

Thematic group: Methods. We present ESR measurements of multiple samples (e.g ruby, Tempol and $Cu(mnt)_2$) using multimode superconducting, inductively coupled $\lambda/4$-resonators, covering both weak- and strong-coupling regimes. These resonators enable microwave spectroscopy from 500 MHz to 20 GHz and down to mK temperatures [1]. At the ESR resonance, we observe pronounced changes in the resonance frequency $f_0(B)$ and a reduction in the quality factor $Q(B)$ of the resonance by up to 100%, reflecting resonant absorption by the spin ensemble. Figure 1 shows this behaviour of $Q(B)$ and $f_0(B)$, stemming from the ESR signal of a Tempol pellet. Additionally $f_0(B)$ also shows typical anti-crossing indicating strong coupling, which is also depicted in figure 2 for the same sample at a different frequency. Here $f_0(B)$ is fitted with the Tavis-Cummings model of a single photon couple to a two-level system [2], obtaining an effective coupling strength Ω of 0.066 GHz.

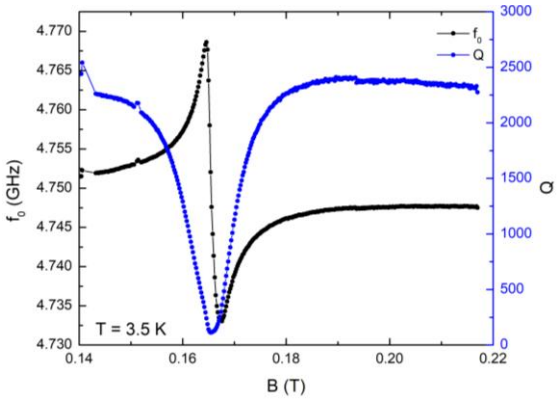

Figure 1: $f_0(B)$ and $Q(B)$ of Nb-resonator with a Tempol pellet on top.

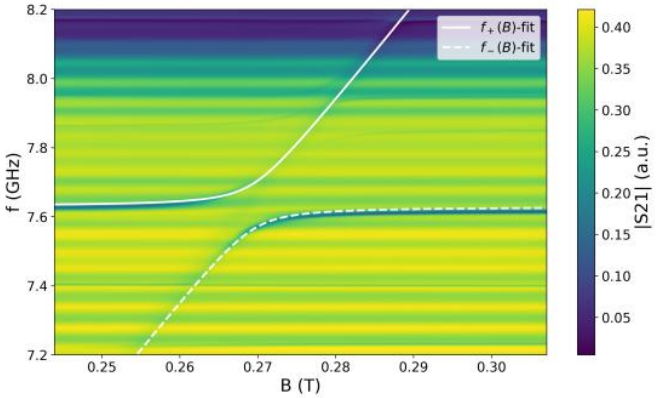

Figure 2: Colormap of $f_0(B)$ of the same resonator as in figure 1, revealing two separate spectral branches as characteristic signature for strong coupling.

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

Nicolai Schröter,[1] Maximilian Hajgel,[1] Marc Henker,[1] Florentine Scharwaechter,[2] Marc Scheffler,[2] Lorenzo Tesi[1]

[1]Institute of Physical Chemistry and Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart, Pfaffenwaldring 55, 70569, Stuttgart, Germany
[2]1st Physics Institute, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

nicolai.schroeter@ipc.uni-stuttgart.de

Molecular Qubits (MQBs) exploit the electronic spin in molecules to access quantum properties, and are investigated towards applications such as quantum computing, quantum sensing, or quantum communication.[1] An interesting case is when such systems have more than two spin levels that can be addressed and manipulated individually. These systems, called Molecular Qudits (MQs), can be based on the hyperfine levels[2] or on multi-spin levels (S=1 or more).[3]

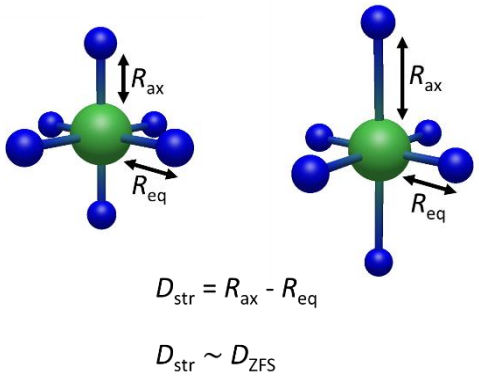

Figure 1. Dependence of the Zero-field splitting in octahedral Ni(II) complexes on the geometry.[5]

However, most of these systems are EPR-silent because they do not show any transition at EPR frequencies that are typical for commercial spectrometers (9 and 35 GHz). In order to investigate MQs it is important to develop new methodologies that allow studying the spin properties of MQs in a broad frequency range. Here, we aim to investigate superconducting on-chip kinetic inductivity detectors (KIDs) to readout the EPR signal of MQs. In principle, these resonators can work at every frequency, can be multiplexed, and their sensitivity can reach the single photon level.[4] Within the project we will design, fabricate and characterize KID resonators, which will then be applied to investigate a series of *S*=1 MQs.

In this specific contribution, I will present the synthesis of a series of *S*=1 Ni(II) octahedral complexes as potential MQs. The zero-field splitting gap of such complexes is very sensitive to the coordination geometry[5] and can be tuned by choosing appropriate ligands (see Figure 1). The characterization of the complexes by SQUID magnetometry, as well as X-band and High Frequency EPR spectroscopy will be presented.

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Resolution Enhancement in Orientation Selective ENDOR – Microwave Chirp Mims ENDOR

Lena Schwieger[1,2], Marvin Lenjer[1,2], Marina Bennati[1,2]

[1] Georg-August University Göttingen, Institute of Physical Chemistry, 37077 Göttingen, Germany; [2] Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany

lena.schwieger@mpinat.mpg.de

Electron paramagnetic resonance (EPR) spectroscopy can be used to investigate the structure and dynamics of paramagnetic centres. An unpaired electron can interact with surrounding nuclear spin, this is called hyperfine interaction. Electron Nuclear Double Resonance (ENDOR) is one hyperfine spectroscopic method. Standard Mims ENDOR consist of a stimulated echo sequence, usually with rectangular pulses, and a selective radio frequency (RF) pulse.[1] One decade ago, arbitrary waveform generators (AWG) became available for EPR instruments, opening the possibility of pulse shaping.[2] Recently, rectangular pulses in ENDOR were replaced by shaped pulses. The implementation of RF chirp pulses in ENDOR pulse sequences increases the sensitivity.[3] Further, replacing MW rectangular pulses with MW chirp pulses results in resolution enhancement in the EPR dimension. This method is called MW chirp Mims (MCM) ENDOR and records the EPR correlated ENDOR spectrum as a function of the RF frequency.[4]

Here, we apply the MCM ENDOR method to a spin system containing two ^{19}F nuclear spin label, resolving the hyperfine structure and chemical shift anisotropy of both nuclear spin label. The experiments are performed on a commercial Bruker E680 W-band (94 GHz) spectrometer.[5] With the MCM ENDOR method, more detailed structure information can be detected allowing benchmarking of DFT calculated parameter. The structure and MCM ENDOR of *o*,*m*-^{19}F nitroxide model system is shown (Figure 1).

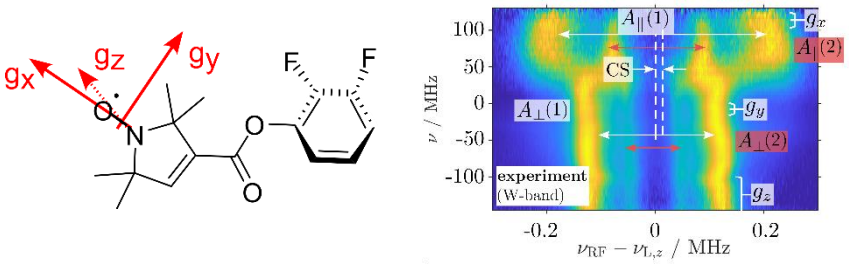

Figure 1: Structure and MCM ENDOR of *o*,*m*-^{19}F nitroxide model system.

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Conformational Dynamics of the Bcl-xL–Bax Interaction in the direct inhibition of apoptosis at the membrane

G.C. Danielle Sedoh,[1] Christina Elsner,[1] Anton Hanke,[2] Francesco Gervasio,[2] Enrica Bordignon[1]

[1] Department of physical chemistry, University of Geneva, [2] Department of Pharmaceutical Sciences, University of Geneva,

e-mail: Gloria.Sedoh@unige.ch

Apoptosis, a form of programmed cell death, plays a pivotal role in balancing cell proliferation to maintain tissue homeostasis, and in the elimination of damaged, or infected cells. It is a highly regulated process and any dysregulation results in pathological conditions including cancer, autoimmune and neurodegenerative diseases. Different pathways can trigger apoptotic cell death with the mitochondrial pathway being the major mode in vertebrates.[1]

This pathway is regulated by the Bcl-2 protein family which comprises promotors (pro-apoptotic proteins) or inhibitors (anti-apoptotic proteins) of cell death.[2] The pro-apoptotic proteins (BH3-only activators such as Bid, Bim, etc. or pore formers such as Bax, Bak) cause pore formation and thus the permeabilization of the mitochondrial outer membrane (MOMP) which is often considered the point of no return of cell death. This process can be inhibited by anti-apoptotic proteins such as Bcl-xL which interact either with activators (indirect mode of action) or with pore formers (direct mode of action). Yet, the mechanism of inhibition, and the structural basis of the inhibitory complexes are still uncertain.

Here we use spin-labeled Bax proteins in Double Electron-Electron Resonance (DEER) spectroscopy to monitor structural changes of the inhibited membrane-bound state. Using SDS-PAGE analysis, we investigate the effects induced by Bcl-xL on the membrane partitioning of Bax at the MOM. Furthermore, combining EPR with molecular dynamics (MD) simulations, we aim to obtain first insights into the inhibitory Bax-Bcl-xL complexes at the mitochondrial membrane to shed light onto the direct mode of inhibition of the MOMP.

This work was supported by SNSF SINERGIA grant CRSII5_216587

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Combining EPR and Solid-State NMR for the Study of Sodium-Ion Storage Mechanisms in Bowl-Shaped Hierarchical Porous Carbon Anodes

Daphna Shimon,[1]

Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel.
Daphna.Shimon@mail.huji.ac.il

There is a growing interest in aqueous sodium-ion batteries, because they offer inherent safety, low cost, and are more environmentally compatible than lithium-ion batteries. As part of this interest, non-graphitizable hierarchical porous carbons have emerged as promising anode materials for sodium-ion batteries. However, the fundamental understanding of sodium storage mechanisms in such complex carbon frameworks remains limited, largely due to the intrinsic structural disorder, heterogeneous porosity, and intricate electronic environments within these materials.

Here, we employ a combination of electron paramagnetic resonance (EPR) and solid-state magic-angle spinning nuclear magnetic resonance (MAS NMR) to elucidate the local chemical environment and dynamics of sodium ions confined within the pores of hierarchical porous carbon frameworks. The hierarchical porous carbon framework contains abundant topological defects, dangling bonds, and turbostratically stacked graphene layers, which give rise to intrinsic paramagnetism and strongly influence Na+ ion–carbon interactions. Moreover, the chemical shifts in MAS NMR directly reflect the interaction of sodium ions with different carbon domains, pore environments, and defect sites. Together, the EPR and NMR results provide a clear picture of the electrical potential-driven Na^+ storage pathway in this energy storage material. These findings provide molecular-level insight into sodium storage in hierarchical porous carbons and offer guidance for the rational design of advanced carbon anodes for aqueous sodium-ion batteries.

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Enhancing EPR Sensitivity Using Cryoprobes and Superconducting Microresonators

G. Usevičius,[1] V. Kalendra,[1,2] I. Pocius,[1] U. Tarvydytė,[1] P. Hogan,[3] A. V. R. de Temino,[3] J.-B. Verstraete,[3] G. A. Jacob,[3] A. Brookfield,[4] A. M. Bowen,[4] B. L. Geoghegan,[5] M. M. Roessler,[5] J. Banys,[1] J. J.L. Morton,[3,6] M. Šimėnas[1]

[1] Faculty of Physics, Vilnius University, Sauletekio 3, LT-10257, Vilnius, Lithuania; [2] Amplify My Probe Ltd., London NW1 1NJ, UK; [3] London Centre for Nanotechnology, University College London, London WC1H 0AH, UK; [4] The National Research Facility for Electron Paramagnetic Resonance, Department of Chemistry and Photon Science Institute, The University of Manchester, Oxford Road, Manchester M13 9PL, UK, UK; [5] Department of Chemistry andCentre for Pulse EPR Spectroscopy (PEPR), Imperial College Molecular Sciences Research Hub London W120 BZ, UK; [6] Department of Electronic & Electrical Engineering, University College London, London WC1E 7JE, UK

mantas.simenas@ff.vu.lt

We discuss recent developments of EPR sensitivity enhancement using X- and Q-band EPR cryoprobes based on fast microwave switches. Such an approach allows us to approach the sensitivity limits of EPR cryoprobes, while maintaining compatibility with commercial spectrometers and conventional samples.[1]

We further present planar high-temperature YBCO superconducting X-band microresonators for measurements of tiny sample volumes. A spiral design provides a microwave mode volume of 7 nL and is integrated into a conventional 3D EPR cavity, ensuring compatibility with existing instrumentation while enabling operation above 1 T and up to 80 K. The microresonator performance is demonstrated by pulsed EPR experiments, including DEER, ESEEM, and ENDOR, achieving spin sensitivity of 10^7 spins/G/√Hz.[2]

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Characterization of vanadium kinetics in redox flow batteries using ultrafast THz rapid-scan EPR spectroscopy

Marc Arvie V. Talavera,[1] Oleksii Laguta,[1] Andriy Marko[1], Miriama Malček Šimunková[1,2] and Petr Neugebauer[1]

[1] MOTES Group, CEITEC-BUT, Purkyňova 656/123, 612 00, Brno, Czech Republic; [2] Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology, Radlinského 9, 812 37, Bratislava, Slovakia

marc.arvie.talavera@ceitec.vutbr.cz

Vanadium redox flow batteries (VRFBs) are promising long duration energy storage technologies for renewable energy sources facilitating the transition from fossil fuels. It maximizes the four existing oxidation states of vanadium, and couples its electrolyte pairs, V(II)/V(III) and V(IV)/V(V), flowing from two external tanks to the anodic and cathodic half-cells of the VRFB, respectively. The charging/discharging cycles drive the reduction-oxidation reactions in the half-cells, during which electrolyte imbalances occur that mainly contributes to battery performance degradation and losses due to, *e.g.*, gas evolution or electrode corrosion over time, requiring an accurate monitoring of electrolyte evolution[1][2]. There is also the challenge coming from the corresponding instrument's time resolution for monitoring as fast kinetics may not be captured from data, losing potentially useful information. Since vanadium (II)-(IV) can possess unpaired electrons, electron paramagnetic resonance (EPR) spectroscopy can be used, specifically applying rapid-scan (RS) EPR technique, where a frequency sweep of up to 10^5 THz/s at fixed magnetic field is performed to emit a transient signal with decreasing oscillation period[2]. This signal undergoes mathematical deconvolution to restore the undistorted EPR spectrum, from which the vanadium concentration can be calculated[2]. This project aims to address this fast kinetics monitoring by designing RS-EPR experimental setups with ultrafast sweep rates for more acquisitions over time in the lower millisecond range, and using higher THz frequencies, as contrast to X-band, to fully characterize V(II) and V(III) due to the additional zero-field splitting terms. Based on the conceptualized vanadium RFB test cell, a dedicated sample holder is developed to allow the insertion of the test cell into the EPR spectrometer. Subsequent measurements will be conducted to investigate and optimize vanadium kinetics from electrolyte-electrode interaction.

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On the Reactivity of N-Centered Radicals - Triarylamines vs Verdazyls: Examples of *In Situ* EPR Kinetic Studies

Ján Tarábek[1]

[1] Institute of Organic Chemistry and Biochemistry ASCR, v.v.i., Flemingovo nam. 542/2, Prague 6 160 00, Czechia

jan.tarabek@uochb.cas.cz

Nitrogen-centered radicals (NCRs) represent a structurally and electronically diverse family of open-shell intermediates whose nature has long rendered their direct detection and kinetic characterization a considerable experimental challenge[1-4]. Stability/Reactivity of those radicals represents a crucial point for their applications especially in material chemistry[2,4] and photochemistry[3,4]. Nevertheless, the investigations are not so much focused on the reactivity of *in situ* (directly within the EPR probeheads) generated NCRs. The actual contribution tries to address the needs of detailed kinetic description (such as rate constants and reaction orders) of radical decays by means of EPR and statistical analysis. Finally, kinetic models of decay for different triarylamine radical cations (generated electrochemically) are compared and radicals are divided into two groups based on the outcomes. Additionally, the latter are compared with those related to heterocyclic NCRs like verdazyls.

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Understanding spin-orbit coupling in Co(II) complexes

F. Torić,[1] L. Androš Dubraja[1], M. Herak[2], N. Novosel[2], I. Petreska[3], K. Molčanov[1], Massimo Cametti[4], Yaakoub Saadallah[4,5], Fatima Setifi[5], D. Žilić[1]

[1] Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia; [2] Institute of Physics, Department for Research of Materials under Extreme Conditions, Bijenička cesta 46, 10000 Zagreb, Croatia; [3] Ss. Cyril and Methodius University in Skopje, Faculty of Natural Sciences and Mathematics – Skopje, Institute of Physics, 1000 Skopje, Macedonia; [4] Department of Chemistry, Materials and Chemical Engineering "Giulio Natta", Politecnico di Milano, Via Luigi Mancinelli, 7, Milano 20131, Italy; [5] Department of Chemistry, Faculty of Sciences Ferhat Abbas University of Sétif 1, 19000 Sétif, Algeria

Email: ftoric@irb.hr

Molecular magnets are an ideal platform for physicists to investigate quantum phenomena at the mesoscopic level. It motivates both, chemists and physicists, to synthesize many interesting and challenging complexes with interesting crystal structures and connect the crystal structure with the magnetic properties in order to tune their properties for applications in memory devices, quantum qubits, spintronics, molecular sensors, etc. The backbone of this tunability of physical properties is understanding how structural features affect magnetic properties, i.e., magnetic interaction parameters.

Among the metals from the 3d group, Co(II) stands as the most interesting from the magnetic point of view, as it has an unquenched orbital angular momentum and strong spin-orbit coupling. Here, we present a detailed magnetic study (EPR, SQUID, AC susceptibility) of the selected Co(II) complexes in a distorted octahedral environment involving oxygen and nitrogen atoms, and aim to establish unexplored quantitative criteria for the relationship between magnetic interactions, anisotropy parameters, and structural features [1]. Understanding how to tune spin-orbit coupling is important as it is a primary origin of magnetic anisotropy, it affects spectroscopic properties and relaxation pathways, key properties underlying potential applications.

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200 ms spin coherence of implanted $^{171}Yb^{3+}$:$CaWO_4$ at a zero-field clock transition

Justinas Turčak,[1] Gediminas Usevičius,[1] Vidmantas Kalendra,[1] Jūras Banys,[1] Philippe Goldner,[2] John J. L. Morton,[3,4] Mantas Šimėnas[1]

[1] Vilnius university, Physics faculty, Saulėtekio al. 9, LT-10222 Vilnius; [2] Chimie ParisTech, PSL University, CNRS, Institut de Recherche de Chimie Paris, 75005 Paris, France; [3] London Centre for Nanotechnology, UCL, London, WC1H 0AH, United Kingdom; [4] Department of Electronic & Electrical Engineering, University College London, London WC1E 7JE, UK

justinas.turcak@ff.vu.lt

Near-surface rare-earth spins can be integrated in hybrid quantum devices,[1] however implantation may cause lattice damage with additional decoherence channels.[2] Recently, it was demonstrated that bulk $^{171}Yb^{3+}$:$CaWO_4$ exhibits a 5 kHz zero-field spin-transition line and 150 ms coherence time.[3] Here, using pulsed ESR, we directly probe the 3083.84 MHz zero-field clock transition of $^{171}Yb^{3+}$ implanted within 500 nm of the $CaWO_4$ surface. The ensemble retains a bulk-like linewidth, indicating negligible implantation-induced broadening. At the clock transition, T_2 increases hundredfold, reaching 200 ms below 3 K without dynamical decoupling. There T_2 saturates due to field-insensitive spin dynamics, most likely direct flip-flops. These results demonstrate that near-surface implantation preserves the narrow linewidth and coherence of $^{171}Yb^{3+}$:$CaWO_4$, supporting coupling to interfaces, such as microwave resonators.

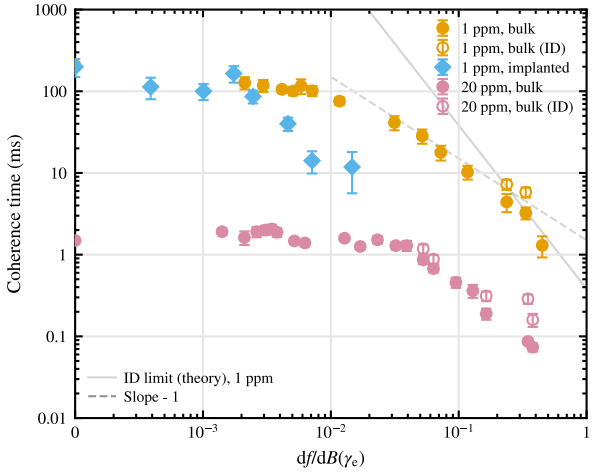

Figure 1: Coherence time enhancement on approaching zero-field clock transition (df/dB = 0).

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Stabilised Peroxyl Radicals and Cold-Plasma-Driven Oxygen Activation at Pyrolytic Carbon–Silica Composites

Dhanalakshmi Vadivel,[1] and Daniele Dondi,[1]

[1] Department of Chemistry, University of Pavia, Viale Taramelli 12, 27100 Pavia, Italy;

dhanalakshmi.vadivel@unipv.it

Understanding the mechanistic evolution of carbonaceous structures during thermal decomposition is essential for optimising pyrolysis-based valorisation routes. We have investigated the nature and reactivity of sp^2 carbons obtained by the pyrolysis of soluble Kraft lignin, a byproduct of the paper-making process. The formation of carbons from Kraft lignin deposited onto high surface-area silica was studied by vacuum pyrolysis at different temperatures, using pristine and acid-washed lignin. Among the various techniques adopted for the material characterization, the Raman measurements showed that the procedure successfully yields carbon atoms organized in sp^2 domains, on the surface of silica, whose dimensions are sub-micrometric. The identification of a very stable peroxyl radical on carbon-modified silica represents a major result, as these species are typically transient. The observed peroxyl radicals are detectable only when both pyrolytic carbon and silica are present. The reactions of pyrolytic carbon onto silica with oxygen and nitrogen monoxide were studied by electron paramagnetic resonance (EPR). The kinetics and reversibility of the reaction with oxygen, as well as the reaction with nitrogen monoxide, were investigated [1]. Furthermore, the prepared carbon material over SiO_2 under cold plasma conditions, the formation of oxygen radicals is increased drastically with respect to the increased irradiation.

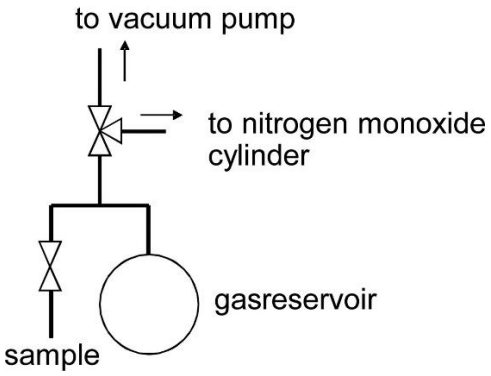

Figure 1: Apparatus for the reaction with nitrogen monoxide

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Unravelling the Role of Structure and Defects in Reduced Commercial Titania with Potential for Visible-Light Photocatalysis

Lore Van den Bergh,[1,2] Sabine Van Doorslaer,[2] Vera Meynen[1]

[1] Laboratory of Adsorption and Catalysis (LADCA), Department of Chemistry, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium; [2] Theory and Spectroscopy of Materials and Molecules (TSM2), Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk, Belgium

lore.vandenbergh@uantwerpen.be

Titanium-dioxide materials are known semiconductors with divers applications in chemical catalysis, the food industry and energy conversion. Several of these applications use the photocatalytic property of titania, which is mostly active in the UV part of the electromagnetic spectrum. By chemically reducing the normally white titania, it can acquire colour, which makes it active in also the visible part of the electromagnetic spectrum [1]. However, in literature there is a lot of contradiction on the most appropriate reduction process and its influence on the properties and photocatalytic activity of the coloured titania. In this project, titania is reduced using a thermal process with $NaBH_4$ as reducing agent [2]. It appears that the reduction is sensitive to many different parameters of the process which are hard to monitor, such as the argon flow or temperature, leading to problems in reproducibility.

In a previous study, another key parameter of reduction, the crystal structure of phase pure titania materials, was investigated, where it was attempted to create a clear overview on the influence of the crystal structure of titania on the reduction. However, it's the more commercially available materials that are of bigger interest to use as photocatalysts, as they are less expensive and more easily available, compared to the very phase pure nanomaterials with specific crystal size. For example, the well-known P25 is often used for its favourable catalytic properties, making it an interesting material to reduce with the intent to even further improve its photocatalytic activity [3]. In this study four commercially available titania materials were reduced and characterized with different spectroscopic techniques, such as EPR, XRD, in-situ drift-FT-IR and UV-Vis DR. EPR, as one of the key techniques reveals insight in the nature of the Ti(III) centres and other defects formed upon reduction of the titania. The effect of the change in crystal structure in the commercial materials is compared with the effect of the reduction on the phase pure samples. Additionally, the effect of other properties, such as crystal size and porosity, on the reduction and vice versa are discussed in this work.

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EPR Studies of Molecular Qubit Assemblies

Joris van Slageren,[1] Jonathan Wischnat,[1] Lorenzo Tesi,[1] Philipp Thielert,[2] Ashley Redman,[2] Johannes Werner,[3] Andreas-Neil Unterreiner,[3] Sabine Richert[2]

[1] Institute of Physical Chemistry, University of Stuttgart; [2] Ulm University; [3] Karlsruhe Institute of Technology

slageren@ipc.uni-stuttgart.de

Paramagnetic molecules that may be employed as molecular qubits have been shown to possess long coherence times in the three digit microsecond regime, in nuclear-spin-poor and dilute matrices, such as doped solids and frozen solutions.[1] To make progress toward implementing quantum technologies with such molecules, a long road lies ahead.

A first step is the preparation of two- and other few-qubit assemblies.[2] This is essential for the implementation of two-qubit gate operations. Ideally, the interaction between the two qubits should be switchable, e.g., by light excitation. To this end, we have prepared dimers of the TEMPO radical which are bridged by anthracene moieties, using different coupling strategies.[3] Time-resolved absorption measurements reveal different intersystem crossing efficiencies. The nature of the photoexcited three-spin system was investigatedted by time-resolved EPR measurements.

For quantum computing and quantum simulation, extended two-dimensional arrays of qubits are required. As a first step in this direction, we have prepared self-assembled monolayers (SAMs) of TEMPO-molecules using a modular approach.[4] Careful analysis demonstrated clean SAM formation. EPR measurements on intact SAMs revealed sizable coherence times. Recent investigations with other radicals substantiated and enhanced on these findings.[5]

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Spin-Lattice Relaxation of Impurities in Semiconductors at High Magnetic Fields

Johan van Tol,[1]

[1] National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL;

vantol@magnet.fsu.edu

Defects in materials with sparse nuclear spin environments can exhibit exceptionally long coherence times, making them attractive platforms for quantum computing and quantum sensing. Here we report instead on the spin-lattice relaxation of several spin systems at high frequencies. The multi-frequency pulsed EPR spectrometer at the Maglab is especially suited to investigate the relaxation of spins or spin-qubits as a function of the magnetic field and frequency in the 4-12 Tesla range.

We report on the S=1/2 shallow donor spin systems of phosphorus-doped silicon and nitrogen-doped silicon carbide, which are of interest for quantum computation applications due to the long coherence times in these materials. Even though the spin-orbit coupling is relatively small, we show that the coherence time at high fields can be limited due to the single-phonon spin-lattice relaxation process. In SiC in particular we observe a B^{-4} behaviour of the T_1 at low temperatures, resulting in an multiple orders of magnitude change in T1 over a relatively limited field range. The tuning of the T_1 with can also have advantages, as it allows faster 'reset' times of the spin system.

Finally, we compare these results with recent measurements on various other spin systems, highlighting similarities as well as key material-dependent differences in coherence properties and spin-lattice relaxation mechanisms.

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Exploiting the kinetic selectivity of charge pumping in electrically detected magnetic resonance of 4H-SiC MOSFETs

I. Vandevenne,[1] M. Avramenko,[2] E. Goovaerts,[1] P. Moens,[2] S. Cambré,[1]

[1]TSM[2], Department of Physics, University of Antwerp, Belgium; [2]onsemi, Mechelen, Belgium

Ilias.vandevenne@uantwerpen.be

Charge pumping electrically detected magnetic resonance (CP-EDMR) is a powerful technique for identifying paramagnetic defects at the SiC/SiO_2 interface of 4H-SiC MOSFETs [1]. In charge pumping, an oscillating gate voltage periodically fills and empties interface traps, while a spin-dependent recombination current is detected at the body contact, when a trapped hole recombines with an electron at the interface, or vice versa. By combining charge pumping with EDMR, the selectivity of constant amplitude charge pumping can be exploited to disentangle two competing, performance-limiting interface defects in n-channel 4H-SiC MOSFETs under distinct gate bias conditions [2]. Differences in dynamics (signal inversion), hyperfine structure, and *g*-anisotropy enable assignment to distinct paramagnetic centers. To further separate their contributions, trapezoidal gate excitation with independently varied rise and fall times are applied, enabling selective control over hole and electron emission processes. The results show that the negative CP-EDMR signal A (Figure 1; red) strongly depends on the rise time, indicating hole emission dominated kinetics. In contrast, the positive (blue) signal B is almost unaffected. These findings demonstrate that CP-EDMR under asymmetric gate excitation provides a powerful approach for selectively probing multiple defects at the SiC/SiO_2 interface.

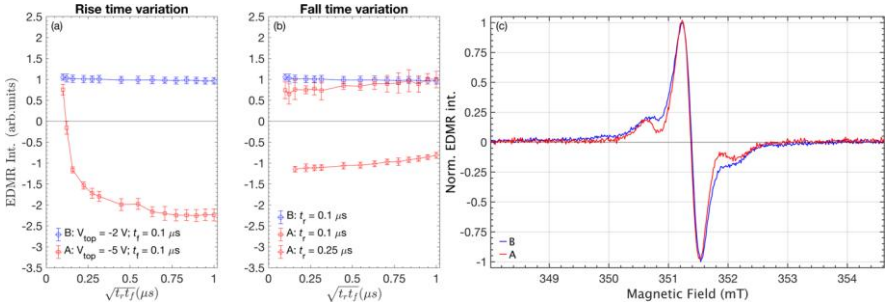

Figure 1: Dependence of the signal intensity on the rise (a) and fall time (b) of signal A (red) and B (blue). (c) Normalized CP-EDMR spectra, at the maximized EDMR intensity.

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Characterization of organic battery materials using in situ UV-visible and EPR spectroscopy

Anatoliy A. Vereshchagin,[1] Oleg V. Levin,[2] Jan Behrends[1]

[1] Berlin Joint EPR Lab, Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany
[2] Electrochemistry Department, St. Petersburg State University, 7/9 Universitetskaya nab., St. Petersburg, Russian Federation

an.vereshchagin@fu-berlin.de

Redox-conductive polymers can be considered as a promising additional energy storage materials due to their high energy density and fast redox kinetics.[1] Understanding their complex dual redox mechanism, involving both polaron/bipolaron and radical transformations, is an intriguing scientific challenge that can aid in the analysis of charge transfer processes. UV-Vis and electron paramagnetic resonance methods (*ex/in situ* cwEPR) offer direct insight into active species, reaction mechanisms, and the local environment of redox centers.[2] Conducting *in situ* electrochemical and spectroscopic experiments is a challenging task due to the structural complexity of the equipment, significant dielectric losses at microwave frequencies when using polar solvents, and the need to maintain an accurate electrochemical potential.

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

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Probing the structural basis for streptococcal rheumatogenicity by pulse dipolar EPR spectroscopy

Katrin Ackermann, Laura Remmel, Hannah M. Weiss, Yichen Wei, Rajni Bala, Bela E. Bode

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

ka44@st-andrews.ac.uk

M proteins are major streptococcal virulence factors involved in a variety of human diseases from mild to potentially life-threatening infections. In addition, some M proteins can induce inflammatory autoimmune conditions like acute rheumatic fever (ARF) and rheumatic heart disease (RHD). The molecular mechanism behind ARF and RHD is not yet understood, partly due to the M proteins evading high-resolution (HR) structural characterisation. M proteins are membrane-anchored at their C-terminus, forming long fibrillar structures consisting of parallel coiled-coil (CC) dimers.[1] While the CC region is conserved to different degrees, the N-terminal region is hypervariable and forms the basis for classification of the more than 275 different emm types.

With no full-length HR structure of any M protein available, AlphaFold (AF) predictions have enabled their study *via* pulse dipolar EPR spectroscopy (PDS). Of special interest for PDS is a highly unusual, predicted fold at the N-terminus of some emm types (coined hammerhead fold due to the reminiscence of the M protein's shape with a hammerhead shark). This fold, in particular the PARF (peptide associated with rheumatic fever) motif,[2] seems to be involved in inducing ARF/RHD through interaction with collagen IV in human cardiac basement membrane.[3]

We have used PDS to experimentally validate the predicted hammerhead fold in full-length rheumatogenic streptococcal M3 protein.[4] We demonstrate that both, the fold and collagen binding capability are lost in a deletion construct lacking part of the fold but still containing the PARF motif. AF modelling combined with multiple sequence alignment suggests that the fold is not unique and may have evolved more than once in streptococci. Understanding the requirements for collagen binding will allow deciphering the pathogenesis of RHD.

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Determination of single-ion anisotropy within the magnetoelectric spin triangle $[Fe_3O(O_2CPh)_6(py)_3]ClO_4 \cdot py$

Abhinav Borbora,[1] Athanassios K. Boudalis[1]

[1] Institut de Chimie de Strasbourg (UMR 7177, CNRS-Unistra), Université de Strasbourg, 4 rue Blaise Pascal, CS 90032, F-67081 Strasbourg, France

borbora@unistra.fr

Molecular spin triangles are examples of geometrically frustrated systems, acting as potential "generalized exchange qubits" for quantum information processing.[1] The homometallic Fe_3 triangle $[Fe_3O(O_2CPh)_6(py)_3]ClO_4 \cdot py$ **(Fe_3),** is a well-studied system of this class, known for its significant magnetoelectric coupling which allows the manipulation of magnetic spin states via electric fields.[2] However, the contribution of single-ion anisotropy arising from each metal center has remain unclear due to the dominance of exchange interactions. This study employs a diamagnetic dilution strategy for the Fe_3 spin triangle system, substituting two Fe(III) ions with diamagnetic Ga(III) ions to isolate and quantify single-ion anisotropy contributions in the $[FeGa_2O(O_2CPh)_6(py)_3]ClO_4 \cdot py$ $FeGa_2$ **(1)** complex. Using X-Band and Q-band EPR at 295 K we extract the single-ion Zero-Field Splitting parameters of Fe(III) within the triangular framework and derive conclusions.

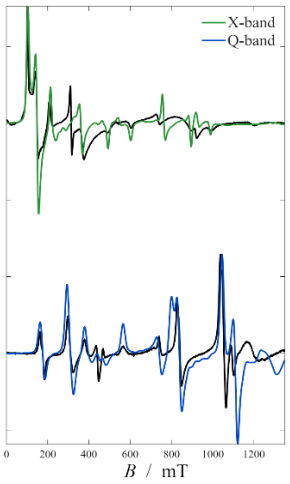

Figure 1: Experimental and simulated EPR Spectra of **(1)** at 295K:

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Physics-Informed AI for Automated Analysis of Dysonian EPR Spectra in Conducting Materials

Dariya Savchenko,[1,2] Andrii Uriadov,[1]

[1] National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Kyiv, 03056, Ukraine;
[2] Technical Center NAS of Ukraine, Kyiv, 04070, Ukraine

d.v.savchenko@kpi.ua

Dysonian lineshapes are commonly observed in EPR spectra of conducting and highly doped materials due to the combined effects of charge-carrier diffusion and the microwave skin depth. Quantitative determination of the resonance field, linewidth, and asymmetry parameters is usually performed using nonlinear least-squares fitting of analytical Dysonian line models. However, such procedures often require careful initialization and may become unreliable in the presence of spectral noise, baseline distortions, or broad resonance lines. We present a physics-informed deep learning approach for automated extraction of Dysonian EPR line parameters. A large synthetic training dataset was generated using physically consistent Dysonian line models for different sample geometries and supplemented with realistic experimental distortions, including noise, baseline variations, and modulation broadening. A one-dimensional convolutional neural network was trained to directly predict the resonance field, linewidth, and the parameter that determines the absorption-dispersion admixture and spectral asymmetry. The method was validated using 195 experimental X-band EPR spectra of Cu-Al-Fe-Mn shape-memory alloy ribbons, highly nitrogen-doped SiC single crystals, and carbon dot-silica nanocomposites. The reconstructed spectra showed excellent agreement with both the experimental data and the parameters obtained using conventional Dyson-line fitting procedures. Compared with MATLAB and EasySpin implementations of nonlinear fitting, the neural-network approach eliminated convergence failures and manual parameter initialization while reducing analysis time by approximately one to two orders of magnitude. The results demonstrate that physics-informed deep learning can provide a fast and robust alternative to conventional Dysonian EPR analysis and offers a practical route toward automated processing of large EPR datasets.

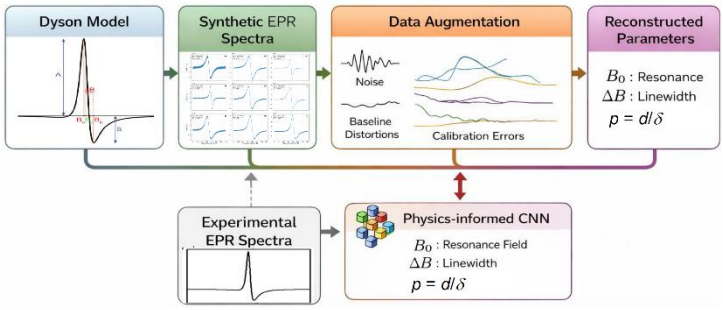

Figure 1: Schematic representation of the proposed physics-informed pipeline for the analysis of EPR spectra with Dyson lineshape.

EFEPR 2026 — Participants / Poster list

First name	Last name	Email	University	Abstract no.
Katrin	Ackermann	ka44@st-andrews.ac.uk	University of St. Andrews	P62
Mikhail	Agrachev	magrachev@ethz.ch	ETH Zürich	CT30
Noorah	Akram	noorahakram20@gmail.com	Government College University Lahore	
Hajar	Amal	hajar.amal@chemie.uni-halle.de	Martin-Luther-Universität Halle-Wittenberg	P1
Stephany Natasha	Arellano Ahumada	torchynsnat@yahoo.com.mx	Instituto Politécnico Nacional	P2
Daina Dayana	Arenas Buelvas	arenas@vutbr.cz	Central European Institute of Technology	yCT1
Dmitry	Azamat	dmitry.azamat@tu-dortmund.de	Technische Universität Dortmund	P3
Paola	Barbara	Paola.Barbara@georgetown.edu	Georgetown University	CT1
Yasmin	Ben-Ishay	Yasmin.ben-ishay@weizmann.ac.il	Weizmann Institute of Science	CT2
Robert	Bittl	robert.bittl@fu-berlin.de	Freie Universität Berlin	PL1
Aharon	Blank	ab359@tau.ac.il	Tel Aviv University	CT3
Dominika	Blicharska	dominika.1.blicharska@student.uj.edu.pl	Jagiellonian University	
Bela	Bode	beb2@st-andrews.ac.uk	University of St Andrews	CT4
Alexey	Bogdanov	alexey.bogdanov@weizmann.ac.il	The Weizmann Institute of Science	CT5
Abhinav	Borbora	borbora@unistra.fr	University of Strasbourg	P63
Athanassios	Boudalis	bountalis@unistra.fr	Institut de Chimie	KE6
Alice	Bowen	alice.bowen@manchester.ac.uk	The University of Manchester	
Paolo Cleto	Bruzzese	paolocleto.bruzzese@unito.it	University of Turin	CT6
Martin	Buhlmann	martin.buhlmann@medizin.uni-leipzig.de	Leipzig University	P4
Camille	Camescasse	ccamescasse@ethz.ch	ETH Zürich	P5
Saverio	Canu	saverio.canu@postgrad.manchester.ac.uk	University of Manchester	yCT2
Aisika	Chakraborty	ac523@st-andrews.ac.uk	University of St Andrews	yCT3
Xiangan	Chen	cxa@ciqtek.com	CIQTEK	

Maria	Chrysina	m.chrysina@inn.demokritos.gr	National Centre for Scientific Research "Demokritos"	CT7
Alberto	Cini	alberto.cini@unifi.it	University of Florence	CT8
Susanna	Ciuti	susanna.ciuti@manchester.ac.uk	The University of Manchester	CT9
Paweł	Czechowski	czechowskipawel9@gmail.com	Novilet	
Tomasz	Czechowski	t.czechowski@novilet.eu	Novilet	CT35
Pranjit	Das	pranjit.das@uni-leipzig.de	Leipzig University	P6
Pedro Henrique	de Oliveira Santiago	pedrophs.santiago@gmail.com	Central European Institute of Technology	P7
Antareekshya	Deka	antareekshya.deka@uni-leipzig.de	Leipzig University	P8
Rajesh	Desapogu	Rajesh.DESAPOGU@um6p.ma	Mohammed VI Polytechnic University	
Anuj	Dhiman	dhiman@ifmpan.poznan.pl	Faculty of Physics and Astronomy, Adam Mickiewicz University	P9
Paul Vianel	Djaba	paul.vianel-djaba@um6p.ma	University Mohammed VI Polytechnic	P10
Eliska	Dolejsova	eliska.dolejsova@ceitec.vutbr.cz	CEITEC BUT	P11
Daniele	Dondi	daniele.dondi@unipv.it	University of Pavia	P12
Pierre	Dorlet	pierre.dorlet@cnrs.fr	CNRS	
Martin	Dressel	dressel@pi1.physik.uni-stuttgart.de	Universität Stuttgart	CT32
Thierry	Dubroca	dubroca@magnet.fsu.edu	National High Magnetic Field Lab	CT10
Jan	Dubský	Jan.Dubsky@ceitec.vutbr.cz	Brno University of Technology	CT11
Dana	Dvoranová	dana.dvoranova@stuba.sk	Slovak University of Technology in Bratislava	P13
Dominika	Działkowska	dd309877@student.polsl.pl	Silesian University of Technology	P14
Lisa	Ebo	lisa.ebo@ehu.eus	University of the Basque Country	CT12
James	Eills	j.eills@fz-juelich.de	Forschungszentrum Jülich	PL2
Martyna	Elas	martyna.elas@uj.edu.pl	Jagiellonian University	PL3
Matthias	Elgeti	matthias.elgeti@uni-leipzig.de	Leipzig University	
Emre	Erdem	emre.erdem@sabanciuniv.edu	Sabanci University	KE1
Amirmohsen	Fanisaberi	Amirmohsen.Fanisaberi@ceitec.vut.cz	Brno University of Technology	P15

El Mustapha	Feddi	e.feddi@um5r.ac.ma	Um6p	
Daylin	Fernández Pacheco	daylin.fernandez-pacheco@chemie.uni-halle.de	Martin-Luther University Halle-Wittenberg	P16
Alexander	Fialkov	alex.fialkov@gmail.com	Tel Aviv University	P17
Maria	Fittipaldi	maria.fittipaldi@unifi.it	University of Florence	
Laura	Galazzo	laura.galazzo@phys.chem.ethz.ch	ETH Zürich	KE2
Inés	García-Rubio	inesgr@unizar.es	Instituto de Nanociencia y Materiales de Aragón	
Blaise	Geoghegan	b.geoghegan@imperial.ac.uk	Imperial College London	
Laisvydas	Giriūnas	laisvydas.giriunas@ff.vu.lt	Faculty of Physics, Vilnius University	P18
Darío	González Diez	dargo10@unizar.es	University of Zaragoza	
Buno	Guigliarelli	guigliar@imm.cnrs.fr	Aix-Marseille University	KE3
Suraj	Halder	surajhalder@iisc.ac.in	Indian Institute of Science	P19
Renny	Hall	renny.hall@hallscientific.co.uk	Hall Scientific Ltd.	
Songi	Han	songi.han@northwestern.edu	Northwestern University	KE4
Jean-Gabriel	Hartmann	jg.hartmann@unistra.fr	Institut de Chimie, Université de Strasbourg	CT13
Yu	He	heyu@ciqtek.com	CIQTEK	
Ayala	Hecht	ayalahecht@mail.tau.ac.il	Tel Aviv university	yCT4
Stephen	Hill	shill@magnet.fsu.edu	Florida State University	KE5
Thijmen	Hooft	6044404@mborijnland.nl	mboRijnland	
Martina	Huber	huber@physics.leidenuniv.nl	Huygens-Kamerlingh Onnes Laboratory, Leiden University	KE7
Ivan	Iushin	iushin.ivan.chem@gmail.com	Leipzig University	P20
Jiri	Janosik	jiri.janosik@rohde-schwarz.com	Rohde & Schwarz - Praha, s. r. o.	
Frédéric	Jaspard	frederic.jaspard@bruker.com	Bruker BioSpin	
Gunnar	Jeschke	gjeschke@ethz.ch	ETH Zurich	PL4
Ilia	Kaminker	iliakam@tauex.tau.ac.il	Tel Aviv University	CT14
Hugo	Karas	hkaras@ethz.ch	UNIGE / ETH Zürich	CT15
Julia	Karczewska	jk309903@student.polsl.pl	Silesian University of Technology	
Annemarie	Kehl	Annemarie.kehl@phys.chem.ethz.ch	ETH Zurich	CT16
Melissa	Kemesies	melissa.kemesies@student.uni-halle.de	Martin Luther	P21

			University Halle-Wittenberg	
Michal	Kern	michal.kern@iis.uni-stuttgart.de	Institute of Smart Sensors, University of Stuttgart	P22
Sudipta	Khamrui	sudipta20102@tauex.tau.ac.il	Tel Aviv University	yCT5
Khuram Shehzad	Khan	ks.khan@ssmeridionale.it	Scuola Superiore Meridionale	yCT6
Rüdiger	Klingeler	klingeler@kip.uni-heidelberg.de	Heidelberg University, Kirchhoff Institute for Physics	P23
Daniel	Klose	daniel.klose@phys.chem.ethz.ch	ETH Zurich	
Tilen	Knaflič	tilen.knaflic@silicon-austria.com	Silicon Austria Labs	P24
Kazumasa	Kojima	m255166@hiroshima-u.ac.jp	Hiroshima University	P25
Petr	Kostelník	petr.kostelnik@onsemi.com	ON Semiconductor Czech Republic	
Lucie	Kotásková	Lucie.Kotaskova1@ceitec.vutbr.cz	CEITEC BUT	P26
Jakub	Kovář	247258@vut.cz	Brno University of Technology	P27
Sebastian	Krebs	sebastian.krebs@medizin.uni-leipzig.de	University of Leipzig Medical Center	P28
Eugeny	Kryukov	eugeny@cryogenic.co.uk	Cryogenic Ltd	CT33
Tomasz	Kubiak	kubiakt@amu.edu.pl	Adam Mickiewicz University	CT17
Periannan	Kuppusamy	Periannan.Kuppusamy@Dartmouth.edu	Dartmouth College	KE8
Ilya	Kuprov	ilya.kuprov@weizmann.ac.il	Weizmann Institute of Science	PL5
Sergei	Kuzin	ksvinout@gmail.com	Max Planck Institute for Multidisciplinary Sciences	P29
David	Kučera-Čavara	dakuceracavara@irb.hr	Ruđer Bošković Institute	P30
Oleksii	Laguta	oleksii.laguta@ceitec.vutbr.cz	CEITEC, Brno University of Technology	
Manuela	Liberi	Manuela.Liberi@bruker.com	Bruker	
Lubomir	Loci	lubomir.loci@manchester.ac.uk	University of Manchester	yCT7
Janet	Lovett	jel20@st-andrews.ac.uk	University of St Andrews	
Ivan	Lubar	ivan.lubar@fysik.lu.se	Lund University	
Fernando	Luis	fluis@unizar.es	INMA, CSIC	KE9
Alessandro	Lunghi	lunghia@tcd.ie	Trinity College Dublin	KE10

Sujan	Maity	maity@vutbr.cz	CEITEC BUT	P31
Michal	Malcek	michal.malcek@stuba.sk	Slovak University of Technology in Bratislava	P32
Miriama	Malček Šimunková	miriama.simunkova@stuba.sk	Slovak University of Technology	P33
Shibnath	Mandal	shibnathmandal7663@gmail.com	Indian Association for the Cultivation of Science	yCT8
Alysia	Mandato	Alysia.Mandato@unige.ch	University of Geneva	yCT9
Gianluca	Marcozzi	gianluca.marcozzi@fu-berlin.de	Freie Universität Berlin	P34
Franka	Markić	fmarkic@irb.hr	Ruđer Bošković Institute	P35
Andriy	Marko	andriy.marko@ceitec.vutbr.cz	CEITEC-BUT	
Oleh	Martyniuk	martyniuk@vutbr.cz	CEITEC VUT	
Jesús I.	Martínez	jimartin@unizar.es	Universidad de Zaragoza	P36
Maximilian	Mayländer	m.maylaender@bruker.com	Bruker	CT34
Dalibor	Merunka	merunka@irb.hr	Ruđer Bošković Institute	P37
Susanne	Mossin	slmo@kemi.dtu.dk	Technical University of Denmark	KE11
Jorge	Navarro-Giraldo	jornagi@uv.es	ICMOL - Institute of Molecular Science	P38
Shoaib	Nazir	comsian.shoaib@gmail.com	Shenzhen University	yCT15
Petr	Neugebauer	neugebauer@vutbr.cz	CEITEC, Brno University of Technology	
Orit	Nir-Arad	oritnir1@mail.tau.ac.il	Tel Aviv University	CT18
Jim	Nolden	6044335@mborijnland.nl	MBO rijnland	
Valentin	Novikov	novikov@ub.edu	University of Barcelona	CT19
Lenka	Novotná	lenkanovotna304@gmail.com	FCHPT STU	P39
Maria Chiara	Pagliero	mariachiara.pagliero@unito.it	Università di Torino	yCT10
Petr	Pelikán	267572@vutbr.cz	CEITEC BUT	P40
Maxence	Perot	maxence.perot@fysik.lu.se	Lund University	
Ivan	Petkov	ivan.petkov@manchester.ac.uk	University of Manchester	yCT11
Aistė	Peštenytė	aiste.pestenyte@gmail.com	Vilnius University	yCT12
Piotr	Pietrzyk	piotr.pietrzyk@uj.edu.pl	Jagiellonian University in Krakow	P41, P43
Ignas	Pocius	ignas.pocius@ff.vu.lt	Vilnius University	P42
Alexey	Popov	a.popov@ifw-dresden.de	Leibniz Institute for	CT20

			Solid State and Materials Research	
Alberto	Privitera	alberto.privitera@unifi.it	University of Florence	CT31
Natalia	Radzikowska	natalia.radzikowska@student.uj.edu.pl	Jagiellonian University	yCT13
Peter	Rapta	peter.rapta@stuba.sk	Slovak University of Technology in Bratislava	P44
Mohamed Amine	Rhanbouri	MohamedAmine.RHANBOURI@um6p.ma	UM6P	P45
Viktor	Rindert	viktor.rindert@ftf.lth.se	Lund University	
Roberto	Rizzato	roberto.rizzato@tum.de	Technical University of Munich	CT21
Maxie	Roessler	m.roessler@imperial.ac.uk	Imperial College London	PL6
Maya	Rämisch	maya.raemisch@mpinat.mpg.de	Max-Planck-Institute for multidisciplinary science	yCT14
Vinicius Tadeu	Santana	santana@vutbr.cz	Central European Institute of Technology - Brno University of Technology	
Takuma	Sato	takuma.sato@cec.mpg.de	MPI CEC	CT22
Dariya	Savchenko	d.v.savchenko@kpi.ua	NTU Kyiv	P64
Florentine	Scharwaechter	florentine.scharwaechter@pi1.uni-stuttgart.de	Universität Stuttgart	P46
Patricia	Schmidt	patricia.schmidt@medizin.uni-leipzig.de	Leipzig University	
Nicolai	Schröter	nicolai.schroeter@ipc.uni-stuttgart.de	University of Stuttgart	P47
Mathias	Schubert	schubert@engr.unl.edu	University of Nebraska-Lincoln	CT23
Lena	Schwieger	lena.schwieger@mpinat.mpg.de	Georg-August Universität Göttingen	P48
Gloria Candy Danielle	Sedoh	Gloria.Sedoh@unige.ch	University of Geneva	P49
Tom	Sertic	snidenevada@yahoo.com	communications & power industries	
Daphna	Shimon	Daphna.Shimon@mail.huji.ac.il	Hebrew University of Jerusalem	P50
Lucca	Sielaff	lucca.sielaff@mpinat.mpg.de	Max Planck Institute for Multidisciplinary Sciences	CT24
Mantas	Simenas	mantas.simenas@ff.vu.lt	Vilnius University	P51

Lorenzo	Sorace	lorenzo.sorace@unifi.it	University of Florence	CT25
Qin	Su	stephen@ciqtek.com	CIQTEK	
Jeff	Sun	xiaxy@ciqtek.com	ciqtek	
Zhiyu	Sun	zhiyu.sun@ciqtek.com	CIQTEK	CT36
Muhammad	Tahsin	tahsin@vutbr.cz	CEITEC-VUT	yCT18
Marc Arvie	Talavera	mavtalavera@gmail.com	CEITEC BUT	P52
Ján	Tarábek	jan.tarabek@uochb.cas.cz	Institute of Organic Chemistry and Biochemistry of the CAS, v.v.i.	P53
Gilles	Thibault	gilles.thibault@bruker.com	BRUKER	
Filip	Torić	ftoric@irb.hr	Ruder Boskovic Institute	P54
Justinas	Turčak	jurcak123@gmail.com	Vilnius University	P55
Dhana-lakshmi	Vadivel	dhanalakshmi.vadivel@unipv.it	University of Pavia, Department of Chemistry	P56
Lore	Van den Bergh	lore.vandenbergh@uantwerpen.be	University of Antwerp	P57
Alex	van der Ham	alexander.van-der-ham@weizmann.ac.il	Weizmann Institute of Science	
Sabine	Van Doorslaer	sabine.vandoorslaer@uantwerpen.be	University of Antwerp	PL7
Joris	van Slageren	slageren@ipc.uni-stuttgart.de	University of Stuttgart	P58
Johan	van Tol	vantol@magnet.fsu.edu	Florida State University - National High Magnetic Field Lab	P59
Ilias	Vandevenne	ilias.vandevenne@uantwerpen.be	University of Antwerp	P60
Anatolii	Vereshchagin	an.vereshchagin@fu-berlin.de	Freie Universität Berlin	P61
Olga	Vojtíšková	olga.vojtiskova@phys.chem.ethz.ch	ETH Zürich	yCT16
Maxim	Yulikov	myulikov@ethz.ch	ETH Zurich	CT26
Michal	Zalibera	michal.zalibera@stuba.sk	Slovak University of Technology in Bratislava	CT27
Roberto	Zambon	roberto.zambon.2@studenti.unipd.it	Università degli Studi di Padova	CT28
Ikram	Zdeg	Ikram.Zdeg@ceitec.vutbr.cz	CEITEC BUT	yCT17
Dijana	Žilić	dzilic@irb.hr	Ruđer Bošković Institute	CT29