47th FGMR Annual Discussion Meeting

International Conference of the German Magnetic Resonance Community

final program and general information

September 14-17, 2026 Mainz, Germany

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

www.gdch.de/fgmr2026

www.fgmr2026.uni-mainz.de/

Division of Magnetic Resonance of the German Chemical Society

Opening remarks and organization

We are delighted to welcome you to Mainz for the 47th FGMR Annual Discussion Meeting, organized by the Division of Magnetic Resonance (FGMR) of the German Chemical Society (GDCh).

This year, we are particularly pleased to host the meeting in close collaboration with distinguished colleagues from **Spain and Portugal**, further strengthening the international character of this long-standing forum for the magnetic resonance community.

The scientific program will cover the full breadth of magnetic resonance research, encompassing all fields in which the resonances of electron and/or nuclear spins are detected. Topics will include solution and solid-state NMR and EPR, as well as a broad range of related and emerging areas such as hyperpolarization, molecular dynamics and diffusion, magnetic resonance imaging, instrumentation and methodology, and magnetic resonance in challenging or unconventional systems. As always, we also look forward to contributions spanning the boundaries of established disciplines and showcasing exciting new developments.

The program features three tutorials, 11 plenary lectures, and 23 invited talks, distributed across three parallel sessions. In addition, 25 contributed abstracts will be selected for promoted oral presentations, providing further opportunities for young and established researchers alike to present their latest results to a broad expert audience. Two extended poster sessions will complement the oral program and provide ample time for detailed scientific exchange, discussion and networking.

We hope that the meeting will provide an inspiring and stimulating environment for open discussion, fruitful exchange of ideas, and the establishment of new scientific collaborations. We particularly encourage all participants to engage actively with one another, to share their expertise and perspectives, and to use this opportunity to spark new ideas and help drive innovative developments in magnetic resonance research worldwide.

We are very much looking forward to welcoming you to Mainz and to an exciting, productive, and enjoyable meeting!

Sincerely yours,
The Scientific and Local Organizing Committees

German Scientific Committee

Prof. Dr. Björn Corzilius, University of Rostock
Dr. Guinevere Mathies, University of Konstanz
Prof. Dr. Jörg Matysik, University of Leipzig
Prof. Dr. Ann-Christin Pöppler, University of Würzburg
Prof. Dr. Olav Schiemann, University of Bonn
Prof. Dr. Monika Schönhoff, University of Münster
Dr. Karsten Seidel, BASF SE, Ludwigshafen
Prof. Dr. Thomas Wiegand, RWTH Aachen University

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Prof. Dr. Óscar Millet, CIC bioGUNE, Derio
Prof. Dr. Miquel Pons, University of Barcelona

Portuguese Scientific Committee

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Prof. Dr. Mariana Coutinho Sardo, University of Aveiro

Local Organizing Committee

Prof. Dr. Dmitry Budker (Institute of Physics, JGU & Helmholtz Institute)
Dr. Peter Blümler (Institute of Physics, JGU)
Dr. Raphael Kircher (Helmholtz Institute)
Christine Best (Institute of Physics, JGU)
Dr. Robert Graf (Max Planck Institute for Polymer Research, Mainz)
Dr. Mihail Mondeshki (Institute of Chemistry, JGU)

Gesellschaft Deutscher Chemiker e.V.
(German Chemical Society)

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FGMR organization: Frank Schröpel

Executive Director: Dr. Tom Kinzel
Registered Charity No.: VR 4453, Registergericht Frankfurt am Main

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Prizes and Awards

Felix-Bloch Lecture:

Dr. James Eills

Albert-Overhauser Award:

Dr. Fabian Hecker

Ernst Awards:

Leonardo Levorin

Julius Frederik Matz

Dr. Lennart Wichmann

Otto-Stern Prize:

Prof. Dr. Axel Haase

General Information for Participants

The conference will be held September 14-17, 2026,
at Johannes Gutenberg University Mainz

WEBSITE: https://www.fgmr2026.uni-mainz.de/

Mutual Respect at Conferences

We kindly ask all participants to contribute to a conference environment characterized by mutual respect, inclusivity, and open communication. Please be considerate and respectful in all interactions with fellow participants, speakers, organizers, and staff.

Conference Venue

Johannes Gutenberg University (**JGU**) Mainz
Central Campus
Philosophicum I, Jakob-Welder-Weg 18

A campus map and floor map of the *Philosophicum* is found at the end of this document (page 140 ff) or can be accessed here.

Conference Rooms (see page 140 ff)

Plenary sessions: P1
Parallel sessions: P1, P2, P3
Posters and exhibition: Foyer P2–P5

Conference Office and Information Desk

The Conference Office and Information Desk is located on the ground floor of the *Philosophicum* building (in front of lecture hall P1)

Opening Hours

Day	Opening hours
Monday, September 14	13:00–21:00
Tuesday, September 15	08:00–18:00
Wednesday, September 16	08:00–18:00
Thursday, September 17	08:00–17:00

The local organizers, conference staff, and student assistants can be easily identified by their name tags and yellow T-shirts.
Please do not hesitate to contact the Information Desk (+49 177 6558184) if you need assistance or information about the conference, getting around Mainz, accommodation, restaurants and nightlife, or cultural events and activities.

Conference Fees:

Please pay your fees in advance to GDCh. We will not be able to accept payment at the registration. The only alternative is online payment via the GDCh webpage from your smartphone or laptop.

How to get there?

If you arrive by car:

Please find information on how to reach the conference venue by car, including parking information, on the venue, hotels & travel website. (be aware that there is a limit of 30h/year and license plate)

If you arrive by train (including from the airport / see the warning on page 143)

From **Mainz main station** (German "Hauptbahnhof") you can reach the conference venue by bus or tram. There are two stops at approximately the same distance from the venue:

You can reach the conference site via two (at almost equal distance) bus/tram stops with the following lines **(bold = tram**). (see campus map on page 142).

stop 1 (*"Universität"*): 6, **51, 53,** 54, 55, 56, 57, 58, **59**, 64, 65, 75, 78,79, 630

stop 2 (*"Friedrich-von-Pfeiffer-Weg"*): **51, 53,** 54, 55, 56, 57, 58, **59**, 630
(this stop is a bit closer to the venue)

Timetables can be found here (sorry, the website is only available in German). During normal hours, buses and trams run approximately every 5–10 minutes.

Alternatively, you can use the **Mainz Mobilität app**, available from your usual app store. The app allows you to check connections and also purchase tickets.

Bus/tram tickets:

You do not have to buy a ticket if you are holder of the "*Deutschlandticket*".

For all other passengers, tickets can be purchased in several ways:

- **At ticket vending machines** at Mainz main station at the bus/tram stops. We recommend buying some tickets in advance, as vending machines are relatively scarce and can occasionally be out of service.
- **On the bus or tram**, where you can pay directly by **debit or credit card**.
- **Via the Mainz Mobilität app** (see above). To purchase tickets through the app, open the menu (three bars in the top-left corner), register and verify your email address. The rest of the process is quite intuitive. You can pay either via paypal or credit card.

Presentations / Communication

The conference language is ENGLISH!

Talks

All speakers should first identify time and place (lecture hall P1, P2 or P3) from the program (see page 15ff). They should contact the technical staff in the specified lecture hall during a break, at least 4 hours before your presentation, to upload and test their presentation files or to connect and test their own laptop. The computers in the lecture halls will run Windows 11 and Microsoft PowerPoint.
Please stay in the specified time allowing 5 min for questions. We kindly request the speakers to be present in the rooms 15 minutes prior to the start of the sessions to verify with the chairperson and the technical staff that the presentation is available and to receive an introduction to the facilities in the rooms.

Poster Presentations

All poster sessions will take place in the foyer between lecture halls P2 and P5 (ground floor level of the *Philosophicum* building, see map (page 140/141).
Presenters are expected to mount their posters before their session (slots are available in the morning). Please only use the supplied push pins for mounting your poster (DO NOT USE any adhesive materials). You are kindly requested to remove your presentation after the last poster session (last call: Thursday 10 am). The conference management accepts no liability for the posters.
Poster sessions will be on **Tuesday 15:00-16:40** (**odd poster numbers**) and **Wednesday 15:00-17:00** (**even poster numbers**) in the foyer. (For poster numbers refer to page 86ff).

Internet Access

The University of Mainz is a member of the EDUROAM Union: If your university is also part of it, you can use the University WiFi in all buildings via your own Eduroam access. In addition, you may use the conference WiFi-Account for guests:

Network:	eduroam
identity:	fgmr2026@uni-mainz.de
Password:	zK44HJbLRDwZ
	(trust the certificate)

If you're looking for a quiet place to work with power outlets and WiFi, you'll find several work nooks on the ground and first floors of the *Philosophicum's* main building.

Emergencies

Police: 110 Fire brigade: 112

Catering

During the designated coffee breaks (10-10:30) and the poster sessions: Coffee, tea, cold refreshments, and a selection of sweet and savory snacks, as well as fresh fruit, will be provided free of charge to all FGMR participants during the daily breaks.

Monday's welcome mixer

On Monday, we will have a get-together party after the last talk (around 19:00–19:30). There will be finger food, pretzels with Spundekäs, hot dogs, and free drinks. We will also have live music by *Spontaneous Emission* from the Budker Lab.

We look forward to seeing you there!

Lunch: Mensa / Cafeterias / Restaurants

There are several options for lunch at Johannes Gutenberg University Mainz.

A **special lunch menu** has been arranged at the **Zentralmensa** for all conference participants. The menu includes a starter soup, a main dish with side dish, a salad, and 0.5 L of water or a soft drink. The price is **€ 9.00 per person** and payment is made via a **voucher system**. Lunch vouchers can be purchased **for cash only** at the conference office. We would appreciate it if you could bring small change.

Other Cafeterias on Campus

At all other cafeterias and mensas operated by the Studierendenwerk Mainz, payment is possible either via the **"StudiwerkMainz" payment app** or with a **prepaid guest card**.

The app can be downloaded at www.studierendenwerk-mainz.de/app. Please follow the instructions provided on the website.

Please note that the app must be topped up in advance. This can be done via bank account **up to one week before the conference**, or directly at one of the two vending machines located at the **Zentralmensa** and ***Philosophicum***.

The app can be used at all other cafeterias on campus; however, **guest prices** will apply.

Alternatively, you can use a **guest card**. The card is available from the vending machines or the information desk against a **€ 5 deposit**. Guest cards must be topped up with **cash** (only € 5, € 10 and € 20 bills are accepted) at the vending machines. Please understand that we have no possibilities return change!

Restaurants and Bakery

Alternatively, several restaurants and cafés are located on campus within easy walking distance, including *Baron*, *Diwan*, and *Kulturcafé* (*QKaff*). A bakery shop (*Werner's*) is also available. These venues offer a variety of snacks, meals, and drinks. Please refer to the campus map (page 142) for their locations.

Money – ATM

An ATM is available next to the Zentralmensa. It is located in the blue box to the right of the right-hand entrance (see map page 142) and is operated by Volksbank.

Cloakroom

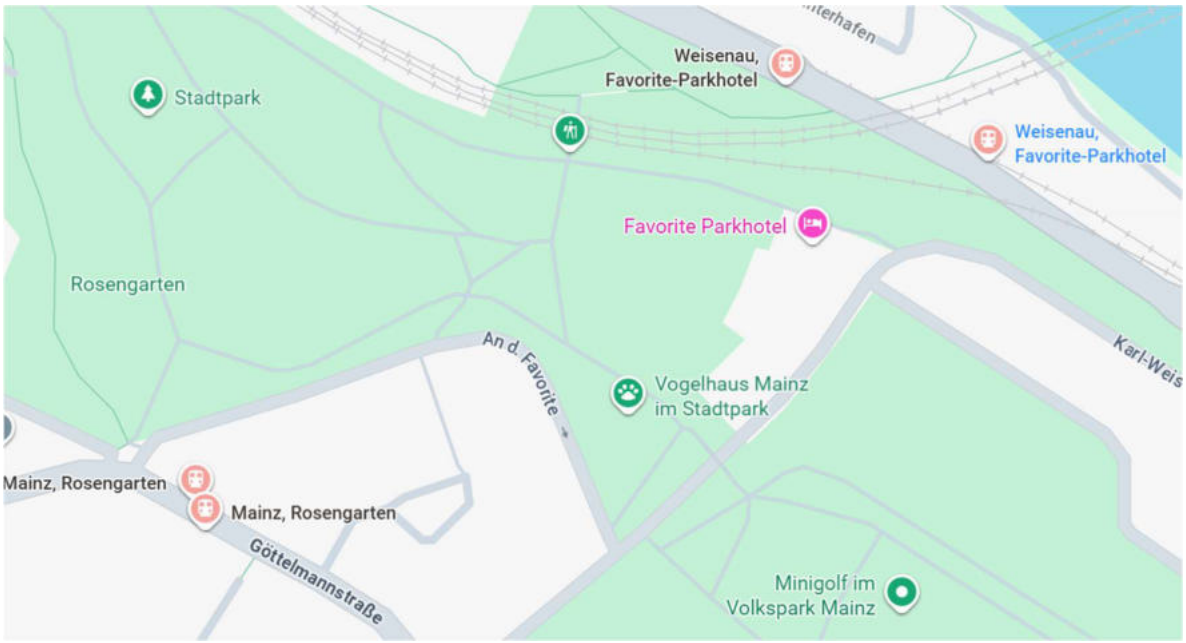
A cloakroom is available for storing coats and luggage on Monday and Thursday. Please contact the information desk for assistance.

Please do not leave any valuables in the cloakroom, as we cannot accept liability for lost or damaged items.

Conference Dinner

The conference dinner will take place on **Wednesday, 16 September, at 19:00** at the Parkhotel Favorite, located in Mainz City Park. The restaurant offers beautiful views over the city and the Rhine River.

Address: Karl-Weiser-Straße 1, 55131 Mainz, phone: +49 6131 80150



How to get there:

There are **two bus stops close to the restaurant**. Unfortunately, there is no direct bus connection from the University, so you will need to change buses in the city center.

The following connections are available between **17:00 and 19:00** from the University main entrance:

1) To Weisenau, Favorite

University main entrance	change at → to	arrival
17:17 line 53	Münsterplatz → 17:27 line 81	17:38
17:28 line 55	Schillerplatz → 17:39 line 63	17:49
17:47 line 53	Münsterplatz → 17:57 line 81	18:08
17:58 line 55	Schillerplatz → 18:09 line 63	18:19
18:17 line 53	Münsterplatz →18:27 line 81	18:38

2) To Mainz, Rosengarten

University main entrance	change at → to	arrival
17:13 line 54	HBF West → 17:19 line 81	17:29
17:28 line 55	HBF West → 17:34 line 62	17:44
17:43 line 54	HBF West → 17:49 line 62	17:59
17:58 line 55	HBF West → 18:04 line 62	18:14
18:13 line 54	HBF West → 18:19 line 62	18:29
18:28 line 55	HBF West → 18:34 line 62	18:44
18:43 line 54	HBF West → 18:49 line 62	18:59

Alternatively: enjoy a walk through Mainz

If you are planning to explore Mainz beforehand, walking to the dinner is also a great option. You can start at the Mainz Cathedral (Dom), walk through the historic old town, and continue towards the excavated Roman Theatre. From the Roman Theatre, the restaurant is only about 1 km (approximately 15 minutes) away, through the beautiful City Park.

Walking route from the Roman Theatre to Parkhotel Favorite

You can plan your city visit by installing the (https://www.mainz.app.de or QR-code) on your smartphone.

(again there seems to be only a German version)

Dinner & Evening Lecture

We will meet at 19:00 on the terrace (if weather permits) for an Apero. After that dinner will be served as a three-course buffet, including one complimentary alcoholic drink. Additional drinks can be purchased at the bar.

Before dessert, we will have an after-dinner lecture by H. W. Spiess (former director of the Max Planck Institute for Polymer Research, Mainz):

“Memories of Giants of Magnetic Resonance”

Taxi Service

You can book a taxis by calling +49-6131-910910 (*Funktaxi*). Please note that you must **specifically request a credit card payment** when booking if you wish to pay by card.

47th FGMR Discussion Meeting 2026 Mainz

(14.9 – 17.9.26 at the JGU, Mainz)

Monday 14th		Tuesday 15th				Wednesday 16th				Thursday 17th			
			Plenary Sessions #1 (P1)				**Plenary Sessions #3 (P1)**				**Plenary Sessions #4 (P1)**		
		8:30	Clement			8:30	Marco-Rius			8:30	Senker		
		9:00	Behr			9:00	Cabrita			9:00	Schmidt-Rohr		
		9:30	Yanai			9:30	Tayler			9:30	Garcia-Rubio		
		10:00	Coffee Break			10:00	Coffee Break			10:00	Coffee Break		
			Awards (P1)				**D) ssNMR: mat/meth(P1)**	**E) HP/NV (P2)**	**F) diff, Scales (P3)**		**J) ssNMR/bio (P1)**	**K) EPR/mat (P2)**	**L) Exotica (P3)**
		10:30	Albert Overhauser Award			10:30	Laurencin	Bucher	Joseph	10:30	Loquet	Risse	Schäfer
		11:00	Ernst Awards			10:55	Hempel	Levien	Stapf	10:55	Marin-Mont.	Van Slage.	Fabricant
						11:15	Krückel	Philipp-Taube	Zankel	11:15	Blokhin	Deka	Breev
						11:35	Mafra	Appelt	Schleicher	11:35	Reif	Schnegg	Wickenbr.
		12:00	**Lunch Break**			12:00	**Lunch Break**			12:00	**Lunch Break**		
13:00	Registration starts		**A) Biodyn (P1)**	**B) Imaging (P2)**	**C) Material (P3)**		**G) Bio/Order (P1)**	**H) Mat/Energy (P2)**	**I) EPR/Method (P3)**		**Awards (P1)**		
	Tutorials (P1)	13:30	Sattler	Penn	Wilhelm	13:30	Törner	Lourenco	Vidal-Gancen.	13:30	Otto Stern Award		
14:00	D. Suter „MR without M-field”	13:55	Möller	Lemkuhl	Brunklaus	13:55	Rezael-Gh.	Jovanovic	Das	14:15	Closing Remarks		
		14:15	Etzkorn	Benders	Scheler	14:15	Friedrich	Enninful	McPeak				
		14:35	Diaz Mor.	Faber	Lopez d. A	14:35	Mendes Fer.	Wisser	Kehl				
15:00	Schmieder: „phase cycling“	15:00	**Poster Session 1** (**odd** numbers) & Coffee Break			15:00	**Poster Session 2** (**even** numbers) & Coffee Break						
16:00	J. Schmedt adG: “MR & 3D-print”	16:40	**Vendor Session (P1)**			17:00	Free afternoon Young Scientists (P2): Tassilo Grün (BASF): *Fully automated Structure Elucidation - NMR in industrial research* Subgroup Meetings						
			Plenary Session #2 (P1)										
		17:00	Anders										
	Welcome & Awards (P1)	17:30	Marcelo										
17:30	Conference Opening	18:00	FGMR General Members‘ Assembly (P1)										
18:00	Felix Bloch Lecture					19:00	Conference Dinner Parkhotel Favorite						
19:00	Welcome Mixer (Foyer/Patio)	20:00	AK EPR meeting (until 21:00) (P1)				After Dinner: Spiess: *Memories of Giants of Magnetic Resonance*						

47th FGMR Discussion Meeting 2026 in Mainz

https://www.fgmr2026.uni-mainz.de/

Scientific Program

Monday 14th September

Session	#	Last name	First name	City	Country	Title	Chair
Mon. 14:00-17:00 (P1) Tutorials	T1	Suter	Dieter	Dortmund	DE	Magnetic Resonance without Magnetic Fields	Robert Graf
	T2	Schmieder	Peter	Berlin	DE	Selecting the desired NMR experiment using phase cycling and gradients	
	T3	Schmedt auf der Günne	Jörn	Siegen	DE	3D Printing of Magic-Angle-Spinning Modules	
Mon. 18:00-19:00 (P1)	BL	Eills	James	Jülich	DE	Phase Transitions of Parahydrogen-Polarized Molecules	

Tuesday 15th September

Tue. 8:30-10:00 (P1) Plenary 1 (P1)	1	Clément	Raphaële	Santa Barbara	US	A statistical mechanics framework for predicting finite-temperature paramagnetic NMR Shifts in complex materials	Björn Corzilius
	2	Behr	Volker	Würzburg	DE	Magnetic Moments beyond NMR Magnetic Particle Imaging: Instrumentation and Application	
	3	Yanai	Nobuhiro	Tokyo	JP	Materials Chemistry Bridging Spin Hyperpolarization and Quantum Sensing	
Tue. 13:30-15:00 (P1) Parallel A *Biosystems:Dynamics*	4	Sattler	Michael	Garching	DE	Dynamics and unfolded conformations in regulating protein-RNA interactions	Ricarda Törner
	5	Möller	Heiko	Potsdam	DE	Lanmodulin-derived Cyclic Peptides as Lanthanide Binders	
	6	Etzkorn	Manuel	Düsseldorf	DE	NMR-guided Characterization and Optimisation of DNA Enzymes	
	7	Díaz-Moreno	Irene	Sevilla	ES	When charge rewrites the molecular landscape: protein order, disorder, dynamics and condensation under post-translational control	
Tue. 13:30-15:00 (P2) Parallel B *Spatially Resoved*	8	Penn	Alexander	Hamburg	DE	A Large-Bore Vertical MRI Platform for Process Imaging in Chemical Engineering and Biotechnology	Peter Blümler
	9	Lehmkuhl	Sören	Karlsruhe	DE	Rapid RASER MRI - Imaging without External RF-Excitation	
	10	Benders	Stefan	Hamburg	DE	Model-Based MRI Reconstruction for Chemical Composition Quantification	
	11	Faber	Cornelius	Münster	DE	On the move: MRI single-cell tracking of immune cells in real time	
Tue. 13:30-15:00 (P3) Parallel C *Materials*	12	Wilhelm	Manfred	Karlsruhe	DE	The potential of low-field NMR spectroscopy for polymer characterization	Monika Schönhoff
	13	Brunklaus	Gunther	Münster	DE	'DeadLi' DNP NMR: Expanding the Spectroscopic Toolbox to Probe Li Metal Electrolyte Interphases	
	14	Scheler	Ulrich	Dresden	DE	Improoved ^{19}F decoupling in MAS solid-state NMR facilitating the characterization of perfluorinated and partially fluorinated materials	
	15	López del Amo	Juan	Vitoria-Gasteiz	ES	Solid-State NMR of Buried Interfaces in Next-Generation Batteries: Linking Reactivity, Ion Transport, and Function	
Tue. 17:00-18 00 (P1) Plenary 2	16	Anders	Jens	Stuttgart	DE	Oscillator-Based Magnetic Resonance: From Integrated Sensors to Dead-Time-Free MR	Miquel Pons Valles
	17	Marcelo	Filipa	Caparica, Almada	PT	NMR Insights into Mucin O-Glycosylation: From Biosynthesis and Conformation to Lectin Recognition	

Wednesday 16th September

Session	#	Last name	First name	City	Country	Title	Chair
Wed. 8:30-10:00 (P1) Plenary 3	18	Marco-Rius	Irene	Barcelona	ES	Methods and Applications of Hyperpolarised MR Across Biological Models	Dima Budker
	19	Cabrita	Eurico	Lisbon	PT	NMR Reveals How Ionic Liquids Reshape Protein Folding Landscapes	
	20	Tayler	Michael	Barcelona	ES	Ultralow-Field Magnetic Resonance in Practice	
Wed. 10:30-12:00 (P1) Parallel D *ssNMR: materials*	21	Laurencin	Daniele	Montpellier	FR	From oxygen-17 isotopic labeling to high-resolution ssNMR: recent advances and applications in materials science	Raphaële Clément
	22	Hempel	Günter	Halle	DE	syncDIPSHIFT – a new method for investigating molecular orientations	
	23	Krückel	Tobias	Aachen	DE	Mechanochemical CO_2 Activation by Frustrated Lewis Pairs (FLPs)	
	24	Mafra	Luís	Aveiro	PT	What the Adsorption Isotherm Cannot Resolve: Solid-State NMR and Atomistic Modelling of Confined CO_2	
Wed. 10:30-12:00 (P2) Parallel E *Hyperpolarization*	25	Bucher	Dominik	Garching	DE	Optically addressable spin systems in diamond and proteins for sensing and imaging	Guinevere Mathies
	26	Levien	Marcel	Lausanne	CH	Dye Sensitized ^{1}H and ^{13}C solid-state NMR at High Magnetic Fields	
	27	Philipp-Taube	Florian	Rostock	DE	Site-specific distance measurements using heteronuclear cross-relaxation dynamics under MAS DNP	
	28	Appelt	Stephan	Jülich	DE	RASER as a sensor for chaos, synchrony and self-organized MRI.	
Wed. 10:30-12:00 (P3) Parallel F *Across different Scales*	29	Joseph	Benesh	Berlin	DE	Kinetic asymmetry drives directionality in an ATP-binding cassette transporter	Mirtha Lourenço
	30	Stapf	Siegfried	Ilmenau	DE	How do binary liquids demix in mesopores? NMR and MD applied to silica pores from 4 to 50 nm	
	31	Zankel	Timon	Darmstadt	DE	^{57}Fe NMR is Great – No Irony	
	32	Schleicher	Erik	Freiburg	DE	Quantitative ESR-Based ROS Analysis: From Model Systems to Clinical Monitoring	
Wed. 13:30-15:00 (P1) Parallel G *Biosystems: Order & Structure*	33	Törner	Ricarda	Zürich	CH	How posttranslational modifications shape cell cycle checkpoint proteins – towards integrating structural biology and chemical biology toolsets	Michael Sattler
	34	Rezaei-Ghaleh	Nasrollah	Pavia	IT	Detection of XH-pi Interactions in Intrinsically Disordered Proteins: A Combined NMR and MD/DFT Approach	
	35	Friedrich	Daniel	Cologne	DE	NMR-Guided Discovery of Membrane-Active Antiviral and Antimicrobial Peptides	
	36	Mendes Ferreira	Tiago	Santiago de Compostela	ES	Solid-state NMR Spectroscopy Methods to study Lipid Membranes	
Wed. 13:30-15:00 (P2) Parallel H *Energy materials*	37	Lourenço	Mirtha	Aveiro	PT	From Molecular Interactions to Material Performance: Understanding Porous Materials	Thomas Wiegand
	38	Jovanovic	Sven	Jülich	DE	Advanced NMR Spectroscopy for Electrolysis Applications: An Overview	
	39	Enninful	Henry	Leipzig	DE	Revealing Ion Exchange and Transport Pathways in Hierarchical Porous Carbon Electrodes	
	40	Wisser	Dorothea	Nürnberg	DE	Solid-state NMR spectroscopy for catalysis: New concepts for self-assembling Supported Ionic Liquid Phase catalysts and heterogeneous photocatalysis in real time	
Wed. 13:30-15:00 (P3) Parallel I *EPR: methods & materials*	41	Vidal Gancedo	José	Cerdanyola del Valles	ES	EPR characterization of radical dendrimers for metal-free MRI contrast agents	Thomas Risse
	42	Das	Panjit	Leipzig	DE	Probing Cu^{2+} Dopant Sites in Zn-based MOF-74 via EPR Spectroscopy	
	43	McPeak	Joseph	Hamburg	DE	Relaxation enhancement and electronic structure investigations in transition metal (Cu, Ni, Fe) doped carbon nitride materials	
	44	Kehl	Annemarie	Zürich	CH	Development of EPR and ENDOR analysis methods	

Thursday 17th September

Session		Last name	First name	City	Country	Title	Chair
Thu. 8:30-10:00 (P1) Plenary 4	45	Senker	Jürgen	Bayreuth	DE	High and Selective Ion Conduction in Electrolyte-Host Materials – Investigating Confinement Effects using NMR Crystallography	Luis Mafra
	46	Schmidt-Rohr	Klaus	Waltham	US	Solid-state ^{13}C and ^{15}N NMR of Functional Organic Materials	
	47	Garcia-Rubio	Ines	Zaragoza	ES	Mapping the Weak Structure of Disordered Loops in proteins using DEER-Restrained Ensemble Modelling	
Thu. 10:30-12:00 (P1) Parallel J *ssNMR: biosystems*	48	Loquet	Antoine	Bordeaux	FR	New solid-state NMR approaches to decipher the molecular organization of fungal and yeast cell wall	Tiago Mendes-Ferreira
	49	Marín-Montesinos	Ildefonso	Aveiro	PT	Combining solid-state NMR with surface and imaging techniques to unravel melittin–membrane interactions	
	50	Blokhin	Dimitrii	Dortmund	DE	Integrated Solid-State-to-Solution NMR Assignment and Solvent Accessibility Mapping of Tryptophan Synthase	
	51	Reif	Bernd	Garching	DE	Aggregation kinetics and amyloid fibril structure probed by solution and MAS solid-state NMR spectroscopy	
Thu. 10:30-12:00 (P2) Parallel K *EPR: materials & energy*	52	Risse	Thomas	Berlin	DE	In-situ and Operando ESR in Heterogeneous Gas Phase Catalysis	Olav Schiemann
	53	van Slageren	Joris	Stuttgart	DE	EPR investigations of Molecular Heterogeneous Catalysis in Confined Geometries	
	54	Deka	Antareekshya	Leipzig	DE	Paramagnetically Doped Metal–Organic Frameworks for Dynamic Nuclear Polarization: An EPR Study	
	55	Schnegg	Alexander	Muelheim/Ruhr	DE	Determination of an unusual positive Cu hyperfine coupling in a square-planar copper(II) complex using multi-frequency EPR and W-band TRIPLE spectroscopy	
Thu. 10:30-12:00 (P3) Parallel L *Exotica*	56	Schäfer	Rolf	Darmstadt	DE	The effect of symmetry, vibrational excitation, spin-orbit coupling and hyperfine interaction on electron spin dynamics probed by magnetic deflection experiments	Amit Finkler & Raphael Kircher
	57	Fabricant	Anne	Berlin	DE	Ultralow-field NMR for biological and industrial applications: A tale of two cities	
	58	Breev	Ilia	Kongens Lyngby	DK	Competing Defect Channels in Sequentially Implanted hBN: Nitrogen as a Bright-Vacancy Source and Oxygen as a Parasitic Sink	
	59	Wickenbrock	Arne	Mainz	DE	Zero- to ultralow-field J-spectroscopy with a diamond magnetometer and applications in neurosurgery	

All posters

#	topic	name	initials	title
1	Solution NMR	Ashish	R. C	Dissecting the influence of (multi)phosphorylation and GlcNAcylation on the regulation of phosphatases by proline isomerization within the CTD of RNA polymerase II
2	Solution NMR	Diehl	B. W. K.	qNMR – Eine analytische Alternative zur HPLC in der pharmazeutischen Analytik
3	Solution NMR	Kölsch	S.	Quantum-Mechanical qNMR of Proteinogenic Amino Acids
4	Solution NMR	Kondrateva	A.	In-situ NMR for the investigation of light-controlled anion-binding adaptive supramolecular systems
5	Solution NMR	Linser	R.	Mapping of dynamic allostery within p38 alpha kinase via network analyses and NMR spectroscopy
6	Solution NMR	Mandral	J.	Selective WET Water Suppression Enables Quantitative Benchtop NMR Analysis in Protonated Solvents
7	Solution NMR	Parsons	E. J.	An Investigation into the Standard Addition Method for the Quantification of Commercially Available Essential Oils via qNMR.
8	Solution NMR	Probst	J.	From π-π-stacking to magnetic self-alignment: NMR investigation of concentration-dependent aggregation in a sterically frustrated hexabenzocoronene
9	Solution NMR	Sanchez	M.	Water Determination for Routine Control
10	Solution NMR	Waldthausen	J. V.	Multinuclear study of the correlation between pH and chemical shift in NMR
11	Solution NMR	Wallwitz	B.	SPEAR Me, c-MYC: Toward the Structural Basis of Epigenetic Inheritance
12	Solution NMR	Woordes	Y.T.	Making the INADEQUATE available: Ernst Angle Excitation and Robust 13C,13C Double Quatum Correlation
13	Small Molecules & Metabolomics	Hadwich	W.	Structural characterization of fractionated beech lignin using NMR spectroscopy and ultrahigh resolution mass spectrometry
14	Small Molecules & Metabolomics	Hunscha	T.	Development of a NMR and MS based tool for automated metabolite identification in complex mixtures
15	Pharmaceuticals & Drug Discovery	Bazhenova	S.	NMR-based Studies on the Structure-Activity Relationship of Antimicrobial Peptides
16	Biological Systems & In Cell	Haardt	A.	Quantification of crRNA bound to Cas13a by Pulsed Electron-Electron Double Resonance
17	Biological Systems & In Cell	Heise	H.	Protein unfolding and aggregation at all stages as seen by NMR
18	Biological Systems & In Cell	Neudecker	P.	Impact of Methionine 35 Oxidation on Monomer Conformational Dynamics and Fibril Formation of Amyloid-beta
19	Biological Systems & In Cell	Reuter	A.	Structure of the full-length YopO-SycO complex based on native mass spectrometry and EPR spectroscopy

#	topic	name	initials	title
20	Materi., Catalysis & Energy	Edalat	A.	syncDIPSHIFT – a new method for investigating molecular orientations
21	Materi., Catalysis & Energy	Elam	D.	Polymer Composition of Recycling Feed
22	Materi., Catalysis & Energy	Elyaagoubi	A. M.	Multiscale Transport in Anion Exchange Membranes Probed via Pulsed Field Gradient NMR.
23	Materi., Catalysis & Energy	Geiger	E.	Temperature- and Concentration-Dependent Ion Dynamics in NaPF6-Based Liquid Electrolytes detected by NMR
24	Materi., Catalysis & Energy	Webber	J. B. W.	Lab-Tools NMR techniques to measure porosity of rocks and viscosity of the recovered liquids.
25	Process Monitor., Quality Control	Nestle	N.	Dissolved or not? Low-field NMR relaxation insights into the microscale mobility of polymers in disperse systems
26	EPR/ESR	Buerger	J.	Synthesis and Characterization of a Binding-Activated, Light-Induced EPR Spin Label
27	EPR/ESR	Denysenkov	V.	Improved Sensitivity of EPR and DNP Methods with Homemade Probeheads
28	EPR/ESR	Gurinovich	N.	EPR spectroscopy in the investigation of polyphosphazene-based organic radical batteries
29	EPR/ESR	Hett	T.	Disentangling Spin-Label and Protein Conformations in PDS EPR
30	EPR/ESR	Neuberger	M.	Characterization of 2,7,12,17-tetra-tert-butyl-Porphycene and it's Pd2+ complex: from synthesis to the photoexcited triplet state
31	EPR/ESR	Schank	R.	Electronic Substituent Effects on Pancake Bonding: Solution-Phase Dimerization Equilibria of Phenyl- and Fluorophenyl-Dithiadiazolyl Radicals
32	EPR/ESR	Sun	Z.	Next-Generation EPR: Combining High-Performance Q Band Instrumentation with Artificial Intelligence Enhanced Spectral Processing
33	Diffusion & Imag. (MRI/EPR)	Austrup	B.	Transport Properties of Solvate Ionic Liquids with Water as Co-Solvent
34	Relaxation & Dynamics	Sarwar	I.	Real-Time Multi-Exponential Component Analysis in TD and FFC NMR Relaxometry
35	Relaxation & Dynamics	Pinna	E.	FFC-NMR method for acquision of T1–T2 maps at different relaxa on fields
36	Relaxation & Dynamics	Rößler	R.	Influence of Paramagnetic Relaxation Additives on DNP-enhanced MAS NMR
37	DNP & Hyperpolarization	Bensons	E. R.	Rotational Resonance for the Selective Boost of Spin Diffusion Pathways under Site-Specific DNP
38	DNP & Hyperpolarization	Dogan	A.	Hyperpolarized Xenon as a Quantum Sensor for Dark Matter: The CASPEr-gradient experiment.

#	topic	name	initials	title
39	DNP & Hyperpolarization	Maliaka	O.	Liquefaction of hyperpolarised xenon for dark matter searches
40	DNP & Hyperpolarization	Schleker	P.	Investigating Parahydrogen-Induced Hyperpolarization and Solidification of Biocompatible Molecules
41	DNP & Hyperpolarization	Serger	L.	Sensitivity enhanced solid-state NMR investigations on multi-layered adsorbents
42	DNP & Hyperpolarization	Singh	A.	Following 1H Spin Polarization across Phase Transitions
43	DNP & Hyperpolarization	Uluca-Yazgi	B.	Solid-State NMR measurement of Spin Diffusion and Relaxation for PHIP-Polarized Solids
44	Solid-state NMR	Lamsal	B.	Effect of subsegmental dynamics of PEG on NMR observables
45	Solid-state NMR	Linke	W. R.	Multi-Stimuli Responsive Supramolecular Systems Studied by NMR Spectroscopy
46	Solid-state NMR	Lusky	O. S.	Sidechain-Backbone Connectivity Revealed by Sensitivity Enhanced Time-Shared NMR Spectroscopy
47	Solid-state NMR	Millow	K.	Effects of Microwave Irradiation on Gadolinium doped Bismuth Oxido Nanoclusters in Solid State NMR
48	Solid-state NMR	Rüthing	L.	3D Printing for Applications in Solid State NMR
49	Zero & Low Field	Tratz	J.	Advanced Methods and Applications in 1D and 2D Low-Field NMR Spectroscopy
50	Zero & Low Field	Rajabi	S	Broadband Benchtop NMR Spectroscopy for Research and Industrial Applications
51	Nano & Quantum Sensors	Schmitt	L.	Towards a Compact NV Relaxometry Demonstrator for Clinical EPR Applications
52	Hardware & Miniaturization	Waldecker	M.	A 500 mT Lightweight Nested Halbach Magnet with 10 ppm Homogeneity for Portable NMR
53	Hardware & Miniaturization	Sarwar	I.	Fast Field Cycling Relaxometry: From Molecular Dynamics to Industrial Applications

Lecture Abstracts

Talk:
T1

Magnetic Resonance without Magnetic Fields

Dieter Suter, Dortmund, Germany and Hefei, China

Dieter Suter, TU Dortmund, 44227 Dortmund, Germany and USTC Hefei, China

For many magnetic resonance experiments, high magnetic fields are essential for providing sufficient sensitivity and for separating spectral components. In a few cases, however, low (~ earth field) or ultralow (<< earth field) magnetic fields are more useful and can enable applications that are difficult or impossible in high field environments. The most important enablers for this type of experiments are the preparation of sufficiently large spin polarization and high-sensitivity detection schemes at low frequencies. In both areas, highly innovative tools have been developed that led to a wide range of applications.

Talk:
T2

Selecting the desired NMR experiment using phase cycling and gradients

P.Schmieder, 13125 Berlin

Dr. Peter Schmieder, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Robert-Rössle-Str. 10, D-13125 Berlin, Germany

NMR spectroscopists have a large variety of experiments at their disposal to extract useful information from a sample and to obtain a structure verification, structural, thermodynamic and kinetic parameters. All these experiments use RF pulses and often gradients to achieve their objective and it is vital to choose the proper combination of those tools to be able to obtain the desired result.

To be able to understand or design an experiment, the concepts of coherence and more importantly coherence transfer pathways need to be understood first. For every experiment there is a desired coherence transfer pathway and it forms the foundation to choose the right combination of pulse phases and gradients.

The necessary phases in an experiment can be derived from the coherence transfer scheme using some simple rules, in the same way the proper strength of the utilized gradients can be calculated.

The concepts of coherence transfer pathways, phase cycling and coherence selection using gradients will be explained (mostly using the product operator formalism), in addition to the tools used to select a particular coherence transfer pathway the experiments NOESY, DQF-COSY, HMQC and HMBC will be discussed.

Literature:

[1] https://www.schmieder-nmr.de/teaching/educational_seminars.htm

[2] https://www.schmieder-nmr.de/teaching/greater_bay_area/greater_bay_area_scripts.htm

Tutorial Talk: 3D Printing of Magic-Angle-Spinning Modules

Lukas P. Rüthing, 57076 Siegen, Ke Xu, 57076 Siegen, Jörn Schmedt auf der Günne, 57076 Siegen, University of Siegen, Faculty IV: School of Science and Technology, Department for Chemistry and Biology, Inorganic Materials Chemistry and Center of Micro- and Nanochemistry and (Bio)Technology (Cμ), Adolf-Reichwein Straße 2, 57076 Siegen, Germany. E-mail: gunnej@chemie.uni-siegen.de

Magic Angle Spinning (MAS) components in general need high precision in manufacturing of the essential components including rotor, stator and caps, which presupposes special equipment and well trained staff and justifies product prices scaling almost linearly with the achievable spinning speed. The advent of additive manufacturing has changed the situation so that MAS components [1] can now be produced in regular NMR groups requiring only minimal investment into a 3D printer and an interested PhD student.
The target of this presentation is to give an introduction into the background of 3D printing, the advantages and disadvantages of different printing techniques, required steps, some advise to avoid common pitfalls in 3D printing, highlight different milestones [1–3] and finally present applications of 3D techniques of pneumatically driven MAS modules and parts for MAS stator/rotor modules in NMR. The presentation is meant to provide the knowledge for getting started with 3D printing of MAS modules.

[1] K. Xu, O. Pecher, M. Braun, J. Schmedt auf der Günne, J. Magn. Reson. (2021) 107096.
[2] K. Xu, F. Aldudak, O. Pecher, M. Braun, A. Neuberger, H. Foysi, J. Schmedt auf der Günne, Solid State Nucl. Magn. Reson. 126 (2023) 101884.
[3] P. Chen, B.J. Albert, C. Gao, N. Alaniva, L.E. Price, F.J. Scott, E.P. Saliba, E.L. Sesti, P.T. Judge, E.W. Fisher, A.B. Barnes, Sci. Adv. 4 (2018) eaau1540.

Phase Transitions of Parahydrogen-Polarized Molecules

A. Singh, Jülich/DE, J. Li, Jülich/DE, B. Uluca-Yazgi, Jülich/DE, P. Schleker, Jülich/DE, J. Eills, Jülich/DE

Dr. James Eills, Forschungszentrum Jülich, 52428 Jülich, DE

Parahydrogen-induced polarization (PHIP) is a fast and inexpensive way to hyperpolarize nuclear spins in molecules. In favourable cases, polarization levels can be high: we routinely produce [1-^{13}C]fumarate with over 30% polarization on the ^{1}H spins, or up to 50% polarization on ^{13}C. At modest concentrations (>10 mM), the sample's internal nuclear-spin dipolar field (the so-called *distant-dipolar field*) can exceed 100 nT, which disrupts the pulse sequences used to generate hyperpolarization and makes dipolar decoupling necessary in liquid-state NMR experiments.[1] PHIP provides a convenient way to access this high-magnetization regime, since it operates at ambient conditions, and experiments are repeatable every few minutes.

In my lab we are investigating liquid-solid phase transitions of hyperpolarized molecules. Initially this provided a convenient way to purify hyperpolarized metabolites via recrystallization,[2] but the solid state offers two other distinct advantages:

- The fixed dipolar couplings allow polarization to diffuse from a hyperpolarized source molecule onto neighbouring target molecules via spin diffusion, offering a potential route to polarizing species that cannot themselves be hydrogenated.[3]
- Relaxation is also much slower, especially at cryogenic temperature, which raises the prospect of storing and transporting hyperpolarized contrast agents.[4]

But these phase transitions present a challenge: as the sample transitions between liquid and solid it passes through the "valley of death", where the molecular tumbling rate equals the Larmor frequency, and T_1 times can be very short. This is a challenge whether freezing or using solvent-based precipitation. We have previously shown that ^{13}C polarization survives acid-induced precipitation of [1-^{13}C]fumarate.[2,3] We are now observing these precipitation processes in real time, and understanding the factors that determine how much ^{1}H, ^{13}C and ^{15}N polarization survives phase transitions for different precipitation approaches.

Literature:

[1] L. Dagys, M. C. Korzeczek, A. J. Parker, J. Eills, J. W. Blanchard, C. Bengs, M. H. Levitt, S. Knecht, I. Schwartz, M. B. Plenio, *Sci. Adv.* 10, eado0373 (2024)

[2] S. Knecht, J. W. Blanchard, D. Barskiy et al., *Proc. Natl. Acad. Sci. U.S.A.* 118, e2025383118 (2021)

[3] M. Gierse, L. Dagys, M. Keim, S. Lucas, F. Josten, M. B. Plenio, I. Schwartz, S. Knecht, J. Eills, *Angew. Chem. Int. Ed.* 63, e202319341 (2024)

[4] A. Capozzi, J. Kilund, M. Karlsson, S. Patel, A. C. Pinon, F. Vibert, O. Ouari, M. H. Lerche, J. H. Ardenkjær-Larsen, *Commun. Chem.* 4, 95 (2021)

Talk:
1

A statistical mechanics framework for predicting finite-temperature paramagnetic NMR Shifts in complex materials

R. Clément,[1,2,3] E. Bassey,[1,2] E. Sebti,[1,2], A. Van der Ven[1]

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[3]Max Planck Institute for Solid State Research, Stuttgart 70569, Germany.

Paramagnetic NMR spectroscopy provides a sensitive probe of local structure and electronic interactions in materials containing open-shell ions, but interpreting the resulting large Fermi contact shifts can be challenging in chemically and magnetically complex systems. Here, we introduce an *ab initio* framework that combines cluster expansions of unpaired electron spin density and magnetic interactions with Monte Carlo sampling to predict finite-temperature paramagnetic NMR shifts. [1] We apply this approach to ^{7}Li and ^{17}O Fermi contact shifts in Li_2MnO_3, a model layered oxide cathode for Li-ion batteries. For both nuclei, the calculated shifts are dominated by chemical site occupancy and magnetic fluctuations, with atomic displacements providing a smaller contribution. Unlike mean-field approaches, Monte Carlo sampling explicitly captures the thermal evolution of local magnetic configurations. The resulting room-temperature shifts show improved agreement on average with experiment, for both ^{7}Li and ^{17}O, highlighting the importance of local magnetic correlations and fluctuations in describing paramagnetic NMR shifts. While further developments are needed for fully quantitative predictions, this framework provides a computationally tractable route to interpreting paramagnetic NMR spectra in chemically and magnetically disordered materials.

Literature:

[1] E. Bassey, *J. Am. Chem. Soc.,* in press (2026).

Talk:
2

Magnetic Moments beyond NMR
Magnetic Particle Imaging: Instrumentation and Application

V.C. Behr, Würzburg/DE

Prof. Dr. Volker C. Behr, Experimental Physics 5,
University of Würzburg, Am Hubland, 97074 Würzburg/DE

Magnetic Particle Imaging (MPI) [1] is an emerging imaging modality that employs magnetic nanoparticles (MNPs) as tracers to determine their spatial distribution and magnetic relaxation properties. While the spatial distribution enables high-resolution imaging, the relaxation behaviour provides access to functional information about the local environment of the nanoparticles. Despite being fundamentally distinct from nuclear magnetic resonance (NMR), MPI shares several conceptual links with NMR, including the use of related or even identical contrast agents, analogous hardware concepts, and overlapping biomedical applications.
The fundamental signal-generation mechanism in MPI is based on the nonlinear magnetic response of MNPs to time-varying magnetic fields. This response generates higher harmonics of the excitation frequency, whose amplitudes are characteristic of both the magnetic properties of the MNPs and their surrounding environment. Consequently, MPI measurements inherently provide spectroscopic information in addition to spatial encoding.
External offset fields can be employed to extend this spectroscopic capability. An example is Critical Offset Magnetic PArticle SpectroScopy (COMPASS), which has been introduced as a highly sensitive analytical method for applications such as antibody detection [2]. Alternatively, spatially varying magnetic fields can be used for encoding the particle distribution. A wide range of MPI scanner architectures has been developed, encompassing setups from compact handheld devices to large stationary scanners [3]. Furthermore, hybrid systems combining MPI with complementary imaging modalities, e.g., NMR, have been demonstrated.
MNPs are typically coated to ensure biocompatibility and can be further functionalised with specific binding groups, e.g., for antibodies. enabling targeted imaging approaches, for example through antibody binding. This enables highly specific analytic applications. Preclinical studies have demonstrated applications including visualization of first-pass blood flow in the murine heart and detection of particle accumulation at specific binding sites. Initial clinical concepts have included a head scanner designed for use in stroke units and a leg scanner intended for interventional procedures [4].

This presentation introduces MPI, the (superpara-)magnetic nanoparticles employed as tracers, the hardware concepts required, and, finally, applications ranging from spectroscopic analysis of MNP binding states to biomedical imaging including the first reported MPI experiments in living humans [5].

Literature:

[1] B. Gleich et al., Nature 2005, 435(7046),1214-1217. [2] P. Vogel et al., Nat. Commun. 2022, 13(1), 7230. [3] P. Vogel et al., Sci. Rep. 2023, 13(1), 10472. [4] A. Neumann et al., J. Magn. Magn. Mat. 2022, 550, 169037. [5] P. Vogel et al., RöFo 2026.

Talk:
3

Materials Chemistry Bridging Spin Hyperpolarization and Quantum Sensing

Nobuhiro Yanai

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Spin polarization is a powerful concept that bridges magnetic resonance and quantum information science. In NMR and MRI, spin polarization can dramatically enhance detection sensitivity, while in quantum information science it serves as an essential initialization process for quantum computing and quantum sensing. Motivated by this broad significance, we have been developing spin-polarizing molecular materials through materials chemistry approaches. In this talk, I will introduce our recent efforts to design and apply molecular spin systems for hyperpolarized magnetic resonance and quantum sensing.

Our work began with dynamic nuclear polarization using photoexcited triplet states of organic molecules (triplet-DNP). By introducing molecular design and materials chemistry into this method, which has been mainly developed in quantum physics, we have expanded triplet-DNP toward biology-relevant molecules and developed new polarizing systems that can operate without strict dependence on crystal orientation [1,2].

We have further shown that materials developed for triplet-DNP can also serve as quantum sensors based on optically detected magnetic resonance (ODMR) [3,4]. We recently enabled intracellular quantum sensing by developing a molecular quantum nanosensor (MoQN). By encapsulating atomically optimized molecular spin qubits within biocompatible nanocrystals, MoQNs achieve highly uniform spin energy levels and enable room-temperature optical detection of molecular spin states inside living cells. This superior uniformity makes absolute temperature sensing within cells possible, which has been difficult to realize with conventional nanoscale quantum sensors.

I will then show how molecular quantum sensing can be extended into chemically programmable materials. By incorporating photoactive chromophores as components of metal–organic frameworks (MOFs), these MOFs enable spatial organization and chemical accessibility of molecular qubits. This design allows quantum sensors whose spin coherence times respond to surrounding chemical species at room temperature [5]. We have also demonstrated the first example of ODMR in a MOF [6]. Optical spin readout in a MOF paves the way for next-generation quantum sensing applications which leverage bottom-up assembly.

Literature:

[1] Keita Sakamoto, …, Nobuhiro Yanai, *Proc. Natl. Acad. Sci. U.S.A.*, **2023**, *120*, e2307926120.
[1] Keita Sakamoto, …, Nobuhiro Yanai, *Nature Commun.* **2025**, *16*, 10045.
[3] Naoto Matsumoto, …, Nobuhiro Yanai, *J. Am. Chem. Soc.* **2022**, *144*, 18023.
[4] Hitoshi Ishiwata, Jiarui Song, Yoko Shigeno, Koki Nishimura, Nobuhiro Yanai, *Science Adv.* **2026**, *12*, eaeb5422.
[5] Akio Yamauchi, …, Nobuhiro Yanai, *Nature Commun.*, **2024**, *15*, 7622.
[6] Miku Inoue, …, Nobuhiro Yanai, *ChemRxiv*, 10.26434/chemrxiv.15004718/v1

Talk:
4

Dynamics and unfolded conformations in regulating protein-RNA interactions

Michael Sattler[1,2*]

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We combine solution NMR in integrative structural biology with crystallography, cryo-EM, small angle scattering and computational methods to study the dynamics of protein-RNA interactions in RNA processing, including alternative splicing regulation and non-coding RNA pathways [1-3]. The structural understanding is a starting point to identify small molecule inhibitors that modulate these pathways for novel therapeutic approaches.

The lecture will discuss how conformational dynamics can specifically regulate biological activity mediated by a non-canonical Ago2 complex with the RNA binding protein Mex3a and miRNA-126-5p [4]. The tandem KH domains of Mex3a mediate RNA binding and contribute to ternary Ago2/MEX3A/miRNA-126-5p interactions. Using NMR methods we identify and characterize a folding/unfolding equilibrium in the Mex3a KH1 domain, where the presence of an unfolded KH domain population enables phosphorylation and modulation of RNA binding and function.

Literature:

[1] Hipp, C., et al (2025). Molecular mechanisms of biomolecular condensate formation in Drosophila melanogaster siRNA biogenesis. *Nucleic Acids Research*, *53*(14), 1–19. https://doi.org/10.1093/nar/gkaf664
[2] Müller-Hermes, C, et al. (2025). Unique conformational dynamics and protein recognition of A-to-I hyper-edited dsRNA. *Nucleic Acids Research*, *53*(12). https://doi.org/10.1093/nar/gkaf550
[3] Martínez-Lumbreras, S., Morguet, C., & Sattler, M. (2024). Dynamic interactions drive early spliceosome assembly. *Current Opinion in Structural Biology*, *88*, 102907. https://doi.org/10.1016/j.sbi.2024.102907
[4] Santovito, D., et al. (2020). Noncanonical inhibition of caspase-3 by a nuclear microRNA confers endothelial protection by autophagy in atherosclerosis. *Science Translational Medicine*, 12(546), https://doi.org/10.1126/scitranslmed.aaz2294

Talk:
5

Lanmodulin-derived Cyclic Peptides as lanthanide binders

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Sequestering lanthanides from electronic waste or mining waters could be an attractive approach to alleviate the growing demand of these metals. Recently, lanmodulins have been discovered in certain bacteria showing astonishingly high affinities towards lanthanide ions.[1] Furthermore, based on lanmodulin, protein constructs have been designed with even increased affinity.[2] Whether these proteins will be robust enough for recycling applications still needs to be shown, though. In this regard, peptides as recognition structures would have clear advantages. However, translating the exceptional affinity of lanmodulin protein domains to short peptide sequences has remained challenging. Initial studies on linear lanmodulin-derived peptides revealed high flexibility and only moderate binding affinities similar to what was found for calmodulin-derived peptides.[3,4] Therefore, we set out to develop cyclic peptides as the conformational constraints imposed by cyclization may alter their properties compared to linear analogues significantly. Here, we present a systematic NMR investigation of a series of lanthanide-binding cyclic peptides and their complexes with lanthanides. Binding affinities were determined by iTC and TRLFS, and corroborated using NMR titrations. It turned out that conventional NMR approaches relying on NOEs and J-couplings, only, provided limited information about the 3D structure. By incorporating paramagnetic NMR methods, particularly pseudocontact shifts, long-range structural information could be collected and the metal-coordinating environments characterized. Our results provide new insight into the structure-affinity relationships governing lanthanide ion binding by cyclic peptides. This work contributes to a deeper mechanistic understanding and supports the rational design of peptide-based systems for selective lanthanide recognition, separation, and future applications in the circular economy.

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(2) Mattocks, J. A.; et al., Nature 2023, 618 (7963), 87.

(3) Gutenthaler, S. M.; et al., Inorg Chem Front 2022, 9 (16), 4009.

(4) Perevedentseva, Y.; et al., chemrxiv 2025. DOI: 10.26434/chemrxiv-2025-lrfbx.

Talk:
6

NMR-guided Characterization and Optimisation of DNA Enzymes

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DNA enzymes (DNAzymes) are promising catalytic nucleic acids with applications in biosensing, biotechnology, and therapeutics. Despite their functional versatility, progress in improving their catalytic efficiency and substrate selectivity is still largely driven by trial-and-error approaches. A major reason is the limited structural information available for DNAzymes in solution, particularly for transient conformations and metal-ion interactions that are essential for catalysis. As a result, the relationship between sequence, structure, dynamics, and activity remains poorly understood, restricting the rational development of improved DNA-based catalysts.

To address this challenge, we apply solution-state NMR spectroscopy as a tool to directly probe the structural and dynamic features of catalytically active DNA enzymes under their operating conditions. Unlike endpoint activity assays or purely computational models, NMR can capture conformational heterogeneity, folding equilibria, and ion-dependent rearrangements at atomic resolution. This is especially important for DNAzymes, whose function often depends on flexible catalytic cores rather than rigid, well-defined folds.

We combine NMR measurements with functional assays to establish a workflow for the characterization and optimisation of DNAzymes. By identifying structural motifs involved in metal ion coordination and catalytic function, we can pinpoint regions where targeted modifications are most likely to enhance performance. This strategy enables the transition from empirical screening toward structure-guided design.
Here, we report on the power of NMR-guided techniques in respect to RNA-cleaving DNAzymes with therapeutic function [1,2,3], and a novel class of autohydrolytic DNAzymes. Surprisingly, for the latter we discover a minimalistic intrinsically disordered DNA design with exceptional activity and programmable features [4]. Our results further expand our mechanistic understanding of DNA in general and extent the toolkit for functional DNA.

Literature:

[1] Borggräfe et al. (2022) Nature, 601, 144.
[2] Borggräfe et al. (2023) FEBS J, 290, 290.
[3] Schmuck et al. (2024) Nature Communications, 15, 5145.
[4] Hesse et al. (2025) Clinical and Translational Medicine, 15, e70408
[5] Zhang, Schmuck et al. *submitted*.

Talk:
7

When charge rewrites the molecular landscape: protein order, disorder, dynamics and condensation under post-translational control

Prof. Dr. Irene Díaz-Moreno, Institute for Chemical Research – cicCartuja, University of Seville - CSIC, Americo Vespucio. 49, 41092 Seville/ES

Cells must rapidly adapt to changes in their physical and chemical environment. Post-translational modifications (PTMs) provide a powerful mechanism to achieve this by rewriting protein charge, conformation, dynamics and interaction networks.

How PTMs reshape the conformational and electrostatic landscapes of proteins will be discussed, using phosphorylation as an example. In NPM1, tyrosine phosphorylation can either promote unfolding or impair DNA binding, depending on the modified domain, thereby controlling nucleolar–nucleocytoplasmic partitioning through order-to-disorder transitions and modulation of charge-driven phase separation [1,2]. In HuR, phosphorylation remodels protein dynamics and interaction interfaces, promoting oligomerization and cytoplasmic redistribution while preserving stress-granule assembly [3,4]. In TIA-1, phosphorylation instead promotes a disorder-to-order transition through electrostatic inter-domain interactions, facilitating self-association and stress-granule formation [5].

These examples illustrate how PTMs act not simply as molecular switches, but as mechanisms for rewriting the molecular landscape—tuning protein order, disorder, dynamics, interactions and condensation to orchestrate cellular responses to stress.

Literature:

[1] Giner-Arroyo R *et al.*, PNAS *under review*. [2] Rivero-García P *et al.*, Nucleic Acids Res. 2026, 54, gkag165. [3] Baños-Jaime B *et al.*, Nucleic Acids Res. 2024, 52, 8552. [4] Baños-Jaime B *et al.*, Adv. Sci. 2025, 12, e2415566. [5] Velázquez-Cruz A & Sánchez-Pulido D *et al.*, Nature Comm. *under review*.

Talk:
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A Large-Bore Vertical MRI Platform for Process Imaging in Chemical Engineering and Biotechnology

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Nuclear magnetic resonance is a key analytical method in chemistry. Its spatially resolved counterpart, magnetic resonance imaging (MRI), offers a comparable advantage for chemical engineering and biotechnology: without perturbing the system, it can map phases, flow, diffusion, and basic chemical composition, inside otherwise opaque reactors. However, existing MRI hardware forces a choice between vertical microimaging confined to bores on the order of centimetres, and wide horizontal clinical systems incompatible with the tall, gravity-driven columns common to chemical engineering.

This presentation introduces a novel vertical 3.0 T MRI platform that attempts to bridge this divide. Its cryogen-free superconducting magnet is vertically oriented and is mounted with its isocentre 4 m above the floor. Its gradient system reaches 120 mT/m for high-resolution and diffusion imaging and slew rates of 700 T m^{-1} s^{-1} for fast imaging across two operating modes. The birdcage radiofrequency (RF) coil delivers excitation fields up to 35 µT. The system accepts samples up to 400 mm in diameter and 3 m in height, which can be translated through the spherical imaging region of about 260 mm in diameter. Application-specific RF receive arrays of up to 32 channels, built in house for each reactor geometry, enable parallel imaging and compressed sensing to accelerate acquisition. A magnet-attached RF shield lets pumps, stirrers, and flow controllers operate nearby without degrading image quality. The performance of this process imaging MRI platform will be shown across different chemical engineering applications: submillimetre mapping of liquid films in a gas-liquid contactor; fast (20 ms) imaging of multiphase dynamics in fluidised beds, and quantitative three-dimensional velocimetry in reactor models spanning the laboratory bench to the pilot scale in the field of biotechnology.

Talk:
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Rapid RASER MRI - Imaging without External RF-Excitation

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Conventional NMR and MRI rely on radio frequency (RF) pulses to excite nuclear spins and in turn generate NMR signals. These pulses require large high-power RF-amplifiers and cause heat deposition in the tissue, which must be minimized for safety, presenting a growing problem when moving toward ever-higher field MRI. An alternative to external rf-excitation is self-excitation using a RASER (Radiofrequency Amplification by Stimulated Emission of Radiation).[1,2] In a RASER, the nuclear spins undergo a spontaneous transition, without RF excitation, from an over-populated state to a ground state. The required population inversion on the nuclear spin states can easily be provided by hyperpolarization techniques. In this work, we use the RASER approach instead of RF pulses for excitation before image acquisition with conventional EPI encoding. [3]

We recorded ^{1}H RASER MRI images of SABRE-hyperpolarized pyrazine (120 mM) with a large matrix (128x128 pixels) in as little as 78 ms at 500 MHz. An EPI sequence is triggered once a set magnetization threshold is reached to ensure an identical signal level. This triggering is enabled by a lock-in amplifier, which also allows for signal acquisition. In this way, we also recorded a time-series of images using a single bolus hyperpolarized pyrazine highlighting the feasibility of dynamic tracking. The demonstrated approach allows recording MRI scans without transmit-receive electronics of the MRI scanner, which is highly desirable for portable MRI as well as the emerging field of hyperpolarized MRI using, e.g., ^{129}Xe gas or HP ^{13}C labelled biomolecules as molecular tracers and imaging agents.

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Talk:
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Model-Based MRI Reconstruction for Chemical Composition Quantification

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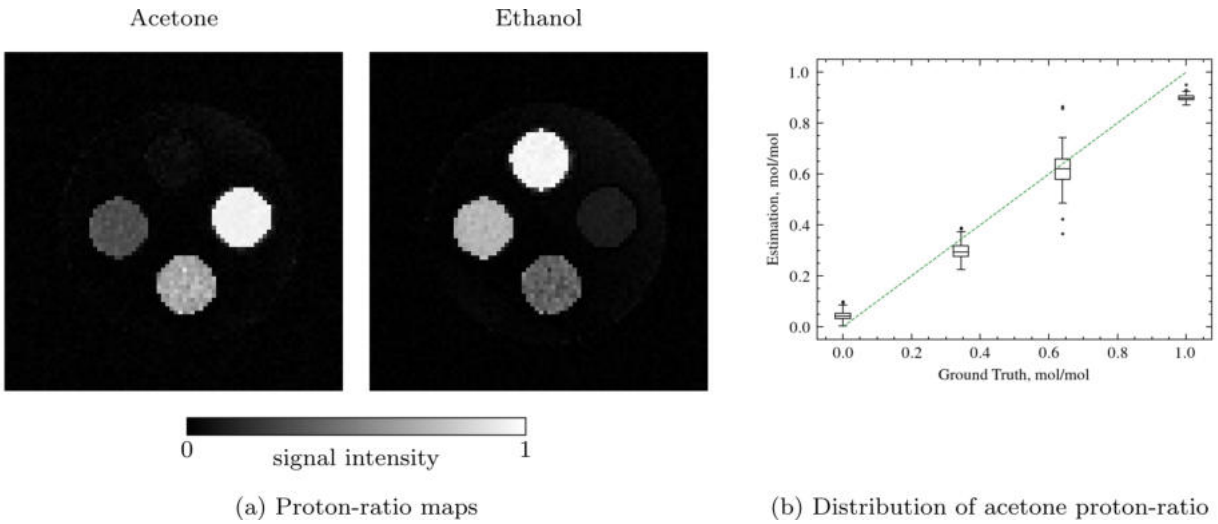
Magnetic Resonance Imaging (MRI) is a powerful measurement technique for chemical engineering applications, enabling the acquisition of phase distributions, flow fields, temperature and many other quantities. As an MR-based technique, MRI is inherently capable of resolving chemical composition. Yet, mapping it remains challenging, primarily due to limitations in spatiotemporal resolution. Recently, von Harbou et al. demonstrated that model-based reconstruction can quantify chemical composition using non-spectroscopic sequences [1]. This approach requires that the components participating in a target reaction be known a priori - typically the case in chemical engineering applications. Consequently, these methods offer a promising framework for monitoring chemical reactions with high temporal resolution.
This work improves upon the foundation of Harbou et al. and expands the method. The acquisition was done using Cartesian multi-gradient echo with acquisition times under 30 s. Application of the method to components with multiple spectral peaks was demonstrated. Furthermore, the model accounts for field inhomogeneities, which are typical for large bore systems such as the one used in this work, increasing accuracy. This represents an important step towards the mapping of chemical reactions in dynamic systems.



(a) Proton-ratio maps (b) Distribution of acetone proton-ratio

Figure: Chemical composition maps of four different acetone and ethanol mixtures.

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Talk:
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On the move: MRI single-cell tracking of immune cells in real time

Cornelius Faber, Münster DE

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Recent advances in magnetic resonance imaging (MRI) have enabled the detection of single cells in vivo, offering a unique opportunity to study cellular behavior in real-time [1-3]. Single cell detection requires labeling cells with superparamagnetic iron-oxide nanoparticles (SPIONs). Both the (bio)chemical (particle coating) as well as the physical (magnetic moment, core size, aggregation state) properties of the SPIONs influence their detectability by MRI. Magnetic field distortions induce a hypointense signal in T2*-weighted images, which ideally allows for the visualization of individual cells in short detection times. The use of time-lapse MRI enables the real-time tracking of labeled cells over time, providing insights into their migration patterns and interactions.

The temporal resolution of time-lapse MRI is the crucial parameter and must be sufficiently high to track certain cell types in real-time, enabling the observation of dynamic processes such as cell migration and interaction with the vascular environment. To increase the velocity detection limit of cells we have recently developed a number of time-lapse MRI sequences. These include both cartesian and radial k space sampling, both 2D and 3D, and, crucially, make use of undersampling schemes [4-6]. Using 3D balanced steady-state free precession (bSSFP) sequences together with compressed sensing reconstruction the whole mouse brain can be imaged at 77 µm isotropic resolution in less than 100 seconds, allowing for the tracking of cells moving at velocities up to 0.8 mm/min [6].

The ability to track single cells in vivo using MRI has significant implications for the study of cellular behavior, particularly in the context of immune cell function and cell-based therapies. We have shown that time-lapse MRI cell count in the brain can serve as a surrogate for detection of inflammation in the body, largely independent of origin or site of inflammation [2,3]. This may help to develop new strategies for diagnostic and therapeutic applications, which underscores the importance of continued innovation in MRI sequence design and image processing methods.

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Talk:
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The potential of low field NMR spectroscopy for polymer characterizatior

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Recent development in high field permanent magnets (based on Nd-Fe-B) allow to conduct NMR spectroscopy in a new and very compact way without the need of liquid N_2 or liquid He. Our group has worked the last 15 years to fully develop the potential of these spectrometers towards polymer characterization including specific hard-ware adaptions. The presentation will cover the basic magnet design and then focus on several polymer related applications.

First, 1D NMR is applied to analysis of polymer pyrolysis oils, where quantification of impurities down to 10 ppm will be demonstrated. Second, SEC is coupled directly on-flow to the NMR spectrometer using cheap protonated solvents, so that chemical composition can be quantified as a function of molar mass. Third, HPLC coupling is discussed. Fourth, 2D NMR methods are applied for analysis in coupled HPLC. Finally, a spectrometer with unique NMR gradient (0.5 T/m) is used to conduct DOSY-NMR, to measure molar mass distribution and chemical composition as a function of molar mass.

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2. M. Matz, et al.; Enhancing sensitivity in the hyphenation of HPLC to benchtop NMR at isoctatic and onflow conditions; *J. Phys. Chem. B* **128** 9512 (2024)

3. M. Gaborieau, et al.; Online coupling of 80 MHz benchtop 2D-COSY NMR to HPLC; *Macromol. Rapid Commun.* 2500239 (2025)

4. J. Tratz, et al.; Potential of Benchtop NMR for the Determination of Polymer Molar Masses, Molar Mass Distributions, and Chemical Composition Profiles by means of Diffusion-Ordered Spectroscopy, DOSY; *Macromol. Rapid Commun.* 2400512 (2024)

5. J. Tratz, et al.; Comparison of different solvent suppression techniques for polymer characterization with a 90 MHz benchtop spectrometer; *Journal of Magnetic Resonance Open* **26** 100213 (2026)

Talk:
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‘DeadLi’ DNP NMR: Expanding the Spectroscopic Toolbox to Probe Li Metal Electrolyte Interphases

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Transport electrification and transition to renewable energy sources demand versatile energy storage opportunities, but next-generation rechargeable batteries with lithium metal anodes in practice are challenged by inhomogeneous Li metal deposition and irreversible losses of Li inventory. [1] This holds in particular for so-called “anode-free” configurations, where the available Li reservoir is limited by the positive electrodes. Despite that some approaches were considered to eventually mitigate irreversible processes occurring upon battery cycling, better understanding of failure mechanisms in cells is required. [2] Analysis based on *in situ* and *operando* NMR may benefit from the quantitative nature of NMR while affording insights upon operation of working cells, as recently highlighted during analysis of complex artificial electrode coatings that eventually bestow better reversibility of Li inventory. [3] Despite that the lifetime of cells is governed by the domain composition and ion transport properties of solid electrolyte interphases (SEI), the actual role of LiF domains present within SEI layers remains controversial as its beneficial impact on electrochemical cycling stability contrasts with its unfavourable intrinsic ionic conductivity.

Here, an optimized ‘DeadLi’ dynamic nuclear polarization (DNP) NMR protocol is introduced, exploiting Overhauser DNP from encapsulated ‘dead’ Li species formed upon cycling to selectively enhance NMR signals of Li metal and adjacent SEI species by up to 80-fold (^{7}Li) at 14.1 T, thereby revealing inverse correlation between Li deposit particle size distribiution, Knight shift reduction, or DNP enhancements, respectively.[4] This enabled morphological assessments of ‘dead’ Li species in ‘anode-free’ lithium metal batteries. DNP-enhanced ^{19}F{^{7}Li} CPMAS, natural abundance ^{6}Li MAS, and ^{6}Li{^{19}F} REDOR experiments were exploited to identify disordered LiF environments in both carbonate/FEC and localized high concentration electrolyte (LHCE) derived SEI layers, consistent with grain boundaries and/or heteroatom-substituted LiF domains rather than the presence of crystalline rock-salt LiF species. Also, REDOR experiments indicated that Li ions traversing LHCE-derived SEIs may interact with more weakly coordinated fluorinated environments than in carbonate-derived SEIs, establishing the introduced ‘DeadLi’ DNP protocol as characterization platform suitable for analysis of interphases of negative battery electrodes, while providing molecular-level insights for a rational design of heterogeneous LiF-based SEIs derived from electrolyte constitutents.

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Talk:
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Improoved ^{19}F decoupling in MAS solid-state NMR facilitating the characterization of perfluorinated and partially fluorinated materials

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Fluorination offers additional functionality in pharmaceuticals and in materials for applications in batteries and in photovoltaics. Fluorine labelling and becomes increasingly used in biomolecular studies.
Fluorine-19 is an ideal probe nucleus for NMR because of its natural abundance of 100%, the highest gyromagnetic ratio next to protons and its very large chemical shift range. In most samples there is no natural background and the background signal from probeheads can be avoided by design. The large chemical shift range means that the signal strongly depends on the chemical environment of the nucleus under study, making ^{19}F NMR a very useful tool. In materials that are only partially fluorinated it does not provide information on non-fluorinated part, then the study of other nuclei like ^{13}C becomes of interest.
The wide frequency span resulting from the large chemical shift range may become challenging for heteronuclear decoupling. Here a new scheme for ^{19}F heteronuclear decoupling based on adiabatic pulses is demonstrated. Supercycled adiabatic pulses improve the decoupling efficiency and thus reduce the ^{13}C linewidth by about a factor of four compared to established phase modulated decoupling schemes or rotor-synchronized π pulses. It is demonstrated by a broadband inversion efficiency of the adiabatic pulses. These adiabatic pulses have proven to be very robust and easy to adjust.
The unprecedented resolution in ^{13}C spectra allows to resolve signals of aliphatic carbons along the fluorinated chain. PVDF is widely used as in membranes or piezoelectric applications. The semicrystalline structure has been intensively studied in ^{19}F solid-state NMR. With the enhanced ^{19}F decoupling combined with ^{1}H the ^{13}C signals from the crystalline part and the amorphous part separated by 1.5 ppm are well resolved and can be assigned by a HETCOR experiment. The signal from the head-to-head polymerizations is shifted by additional 3 ppm and well resolved.
Based on that enhanced resolution the interface of cellulose fibers coated with PVDF are studied and the interface region is selectively excited by short-range cross polarization. Further applications for the study of partially fluorinated proteins and materials are facilitated.

Talk:
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Solid-State NMR of Buried Interfaces in Next-Generation Batteries: Linking Reactivity, Ion Transport, and Function

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Next-generation batteries incorporating solid electrolytes, lithium-metal anodes, and high-capacity silicon electrodes promise increased energy density and improved safety. Their performance, however, is strongly governed by buried interfaces and interphases formed upon contact and during electrochemical cycling. Rational interface design requires identifying the phases that form, establishing whether ions can cross them, and determining how they evolve during operation.

These regions are difficult to characterize because they are often inaccessible, disordered, chemically heterogeneous, and continuously evolving. Solid-state NMR provides local, element-selective information linking interfacial composition and structure to ionic dynamics and electrochemical function. Drawing on our recent work, this contribution illustrates its application across several next-generation battery architectures.

In ceramic–polymer composite electrolytes, exchange NMR reveals lithium communication between inorganic and polymeric phases and shows how ceramic surface chemistry controls interfacial transport.[1] Studies of polymer–sulfide and sulfide–halide combinations identify spontaneous interfacial reactions and their products, while correlation and exchange experiments establish how interphase formation influences lithium mobility and functional compatibility.[2,3] At lithium-metal interfaces, solid-state NMR shows that reduction of a halide electrolyte produces a chemically stratified interphase supporting stable lithium plating and stripping, demonstrating that interfacial reactivity is not necessarily detrimental.[4]

Operando experiments extend this approach by continuously cycling halide- and gel-polymer-electrolyte cells inside the NMR probe while acquiring spectra without interrupting operation. Lithium redistribution, electrolyte consumption, and interphase evolution can therefore be monitored directly during plating and stripping.

Finally, silicon–graphite composite anodes illustrate how electrolyte formulation controls SEI composition, organization, and dynamics and, ultimately, electrode degradation. Exchange measurements further establish spatial relationships between SEI components and lithiated active materials.[5]

Together, these examples demonstrate how solid-state NMR can determine whether buried interphases facilitate ion transport, generate blocking regions, stabilize reactive contacts, or promote degradation, providing essential information for the rational development of next-generation batteries.

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Talk:
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Oscillator-Based Magnetic Resonance: From Integrated Sensors to Dead-Time-Free MR

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Conventional magnetic resonance instrumentation separates radiofrequency excitation and signal detection into distinct transmit and receive paths. While this architecture has enabled highly sensitive and versatile experiments, it also imposes fundamental challenges for miniaturization and for measurements in which spin dynamics evolve during or immediately after excitation. Voltage-controlled oscillators (VCOs) offer an alternative approach: the resonant LC tank simultaneously generates the transverse excitation field and senses the back-action of the spin ensemble, which appears as a modulation of the oscillator amplitude and frequency.

This talk will highlight our recent developments in VCO-based magnetic resonance, spanning chip-integrated NMR transceivers and NMR- and EPR-on-a-chip systems, VCO-enabled approaches to dynamic nuclear polarization (DNP), and oscillator-based detection across a wide range of magnetic-resonance frequencies. Together, these developments illustrate how active resonators can provide not only a route toward compact and scalable MR instrumentation, but also access to measurement modalities that are difficult to realize with conventional transmit/receive architectures.

A particular focus will be on our recent demonstration of phase-coherent pulsed NMR with concurrent excitation and detection. Using an injection-locked VCO array operating around 500 MHz and driving a planar segmented coil, we demonstrate conventional Fourier-transform NMR while continuously observing driven Rabi oscillations during the excitation pulse and the immediate onset of the subsequent free-induction decay. No transmit/receive switch or receiver gating is required. A second VCO-based system operating at 17 MHz further demonstrates phase-coherent multi-pulse operation, including phase-cycled Hahn echo experiments.

In this architecture, the oscillator itself has zero intrinsic dead time because it remains active and sensitive throughout excitation and detection. Residual transients originate from the deterministic response of the phase-locked loop to the frequency switching used for spin manipulation. These transients can be made short compared with relevant NMR timescales and, in principle, removed by deterministic subtraction, enabling continuous recovery of the spin signal across the excitation-to-detection transition.

These results establish oscillator-based detection as more than a strategy for miniaturizing conventional MR hardware. By combining excitation and detection within the same active resonator, VCO-based systems provide a platform for highly integrated and scalable magnetic-resonance sensors and for experiments that exploit uninterrupted access to spin dynamics.

Talk:
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NMR Insights into Mucin *O*-Glycosylation: From Biosynthesis and Conformation to Lectin Recognition

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Mucin glycoproteins participate in fundamental biological processes and contain densely glycosylated domains decorated with structurally diverse *O*-GalNAc glycans [1]. Dysregulation of the glycosyltransferases responsible for their biosynthesis is a hallmark of cancer, leading to tumour-associated glycan epitopes that influence cancer-cell behaviour and immune surveillance [2,3].

The lecture will describe how the group employs complementary ligand- and protein-observed NMR strategies to probe mucin *O*-glycosylation and glycan recognition. NMR spectroscopy, integrated with biochemical and structural biology methods, has enabled us to monitor the modification of MUC1 glycodomains by GalNAc-Ts, C1GalT1 and ST6GalNAc-I, and to determine how peptide sequence, glycosylation-site occupancy and pre-existing glycans regulate enzyme specificity and pathway selection [4-5]. Conformational analysis of mucin *O*-glycopeptides has further revealed how glycan structure and the surrounding peptide sequence shape the molecular presentation of these epitopes. Finally, ligand-observed NMR methods, including STD-NMR and NOESY/ROESY, together with protein-observed chemical-shift perturbation analyses, have provided complementary views of tumour-associated *O*-glycan recognition by immune lectins [6-8]. Collectively, these studies highlight the versatility, robustness and power of NMR for investigating glycan biosynthesis, glycopeptide conformation and lectin recognition within an integrated structural framework.

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Talk:
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Methods and Applications of Hyperpolarised MR Across Biological Models

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The inherently low sensitivity of magnetic resonance (MR) remains one of its main limitations for studying metabolism in live cells. Hyperpolarisation can increase MR signals by several orders of magnitude, enabling the detection of low concentration metabolites and isotopically labelled substrates and, in many applications, the observation of their metabolic conversion in real time. These capabilities have enabled HP-MR to investigate metabolism in living systems across a range of biological models, from cell cultures to animals and patients.

In this talk, I will discuss developments in HP-MR and place our work within the broader evolution of the field. I will focus on how different experimental models can provide complementary information and on the methodological developments required to perform HP-MR measurements across them. In particular, I will present our efforts to integrate HP-MR with advanced *in vitro* models, including 3D cultures and organ-on-chip systems, together with dedicated instrumentation and approaches for increasing experimental throughput [1–3]. I will also discuss applications of these methods to investigate metabolism in disease models *in vitro* and *in vivo*. Finally, I will discuss current challenges in obtaining quantitative, reproducible and biologically meaningful measurements.

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Talk:
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NMR Reveals How Ionic Liquids Reshape Protein Folding Landscapes

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Ion-specific (Hofmeister) effects on protein stability have been recognised since the 19th century, yet their molecular origin remains incompletely understood, particularly regarding the unfolded state. Using imidazolium- and cholinium-based ionic liquids (ILs) as tunable models for ion-specific cosolutes, we previously showed that direct, residue-resolved ion–protein contacts, rather than nonspecific electrostatic screening, govern IL-induced (de)stabilisation of the proteins Im7 and human serum albumin, with anion hydration and cation hydrophobicity both contributing to the net effect [1,2]. Subsequent work on folding-competent model proteins raised a key open question: does the unfolded ensemble itself, and not only the native fold, determine whether an IL stabilises or denatures a protein [3]?

We address this question using the N-terminal SH3 domain of the *Drosophila* adapter protein Drk (drkN SH3), a metastable 59-residue domain that exists in a near 1:1, slow-exchange equilibrium between folded (F) and unfolded (U) states, allowing both conformers to be observed simultaneously by NMR. Site-resolved [^{1}H,^{15}N]-HSQC titrations, temperature-dependent stability curves and ZZ-exchange kinetics show that cholinium glutamate ([Ch][Glu]) and 1-butyl-3-methylimidazolium dicyanamide ([Bmim][dca]) reshape the F/U equilibrium via fundamentally different, entropy-dominated mechanisms. [Ch][Glu] stabilises the folded state (m = +1.9 kcal mol^{-1} M^{-1}), mainly through its glutamate anion, by preferential exclusion from the protein surface that raises the barrier to unfolding (ΔTm up to +20 K) without detectably remodelling the native fold. In contrast, [Bmim][dca] strongly destabilises SH3 (m = –7.7 kcal mol^{-1} M^{-1}) through a markedly non-additive, cooperative action of its cation and anion, which stabilises a non-native α-helical conformation within the unfolded ensemble itself, slowing folding roughly three-fold. This unfolded-state-targeted mechanism is fundamentally distinct from that of classical denaturants such as urea or guanidinium chloride, which instead favour an expanded, random-coil-like unfolded state.

By exploiting the unique ability of NMR to interrogate low-populated and transiently formed protein states at atomic resolution, this work establishes the unfolded ensemble as a critical, previously underappreciated target of ion-specific cosolute action, and provides molecular design principles for tuning protein stability and behaviour with ionic liquids in biocatalysis and protein formulation [4].

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Talk:
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Ultralow-Field Magnetic Resonance in Practice

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Ultralow-field magnetic resonance has a long history, supported by developments in sensitive detection, spin hyperpolarization and magnetic-field control [1]. Our work has pursued two complementary directions within this field: using ultralow magnetic fields to access precise information about spin interactions and dynamics, and developing instrumentation that makes such measurements simpler and more practical. This lecture will discuss recent results from our group along both lines.

Examples will include magnetic resonance imaging at microtesla fields [2], polarimetry studies of hyperpolarized spin systems using atomic magnetometers [3–5], precision spectroscopy, and the development of open-source and integrated magnetic-resonance hardware [6,7]. A recurring theme will be how the choice of NMR instrument architecture determines both the information available from the experiment and the requirements for carrying it out.

I will finish with thoughts on where these developments might take magnetic resonance next.

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Talk:
21

From ^{17}O isotopic labeling to high-resolution ssNMR: recent advances & applications in materials science

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Oxygen is the most abundant element at the surface of our planet, where it is found in both living organisms and inert matter. It is thus no surprise that since the early stages of NMR, efforts have been made to apply instrumental and methodological developments to the study of this nucleus. Yet, the only NMR-active isotope, oxygen-17, suffers from a very low natural abundance (0.04%), making it extremely challenging to investigate.

In 2017, our group in Montpellier proposed a new approach for ^{17}O isotopic labeling using ball-milling [1]. Over the years, we have expanded the number and diversity of molecules and materials labeled by this technique, in order to perform high-resolution ssNMR analyses [2]. In this presentation, after a brief overview of our current state of the art in terms of ^{17}O mechanochemical labeling and ssNMR analyses, we will present some of our most recent results, which include the enrichment of metal carbonate salts, and the study of materials developed for CO_2 capture.

Literature:

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Talk:
22

syncDIPSHIFT – a new method for investigating molecular orientations

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The macromolecules of polymeric materials become partially oriented when the sample is subjected to mechanical loading, such as stretching or compression. The degree of orientation essentially determines the macroscopic properties of the material. To confirm structure-property relations experimentally, absolute values that characterize the degree of chain deformation are required. Anisotropic spin interactions enable NMR investigations in this field. Three conditions must be met in order to estimate the orientation moments of the macromolecular segments: (i) the interaction tensor, including its orientation in the molecule, has to be known; (ii) the interaction anisotropy has to be in the order of the spinning speed required for sufficient spectral resolution; and (iii) the orientation of the specific atomic group within the segment has to be known.

The syncMAS method [1] exploits the chemical shift anisotropy (CSA). For the investigation of oriented polycarbonate (PC), it is not possible to fulfil all three conditions to a sufficient extent: The CSA of the methyl carbons is rather low; the spatial orientation of the aromatic rings is not known with sufficient accuracy and nor is the CSA of the carbonate carbon. Even if syncMAS investigations of PC as described in the literature yield orientation data, the accuracy is rather low for the aforementioned reasons.

One possible solution is an experiment that makes use of the dipolar interactions instead of CSA. The dipolar tensor is determined by the length and direction of the CH bond, thus fulfilling condition (i). The CH dipolar interaction can be monitored site-selectively using the 2D DIPSHIFT pulse sequence [2]. The dipolar information is contained in the curves between the rotational echoes in the indirect dimension. We combined this with rotor synchronization for a 3D experiment in which the time dimension t_2 gives the length of the Lee-Goldburg (LG) decoupling, while t_3 passes during data acquisition. t_1 is proportional to the angle between the sample director and the plane spanned by $\mathbf{B}_0$ and the rotor axis at the start of the pulse sequence. The dependence on t_1 provides information about the sample orientation. This feature is most prominent when the LG decoupling is completely halfway between the rotation echoes, for example when $t_2 = T_{rot}/2$. Fixing this allows us to reduce the experiment to two dimensions. Condition (ii) can also be satisfied. We defined the segment vector as being normal to the $C(CH_3)_2$ plane. Based on this, we determined the orientation moment of the segments. As an additional benefit, information about molecular geometry (ring rotation angles) is obtained.

This method appears to be particularly well-suited to investigating aliphatic carbons.

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Talk:
23

Mechanochemical CO_2 Activation by Frustrated Lewis Pairs (FLPs)

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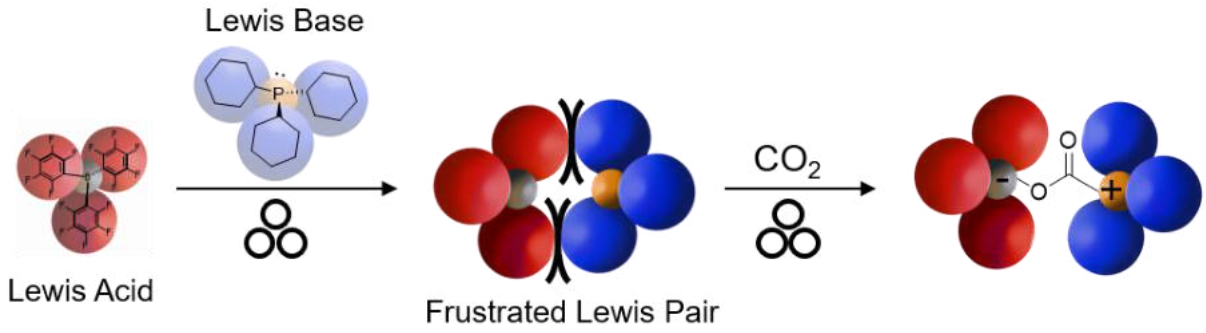
Frustrated Lewis pairs (FLPs) are combinations of a Lewis acid and base, which due to steric hindrance are unable to form a classical acid–base adduct. This 'frustration' leads to unusual reactivity, which has been successfully used for amongst others the activation of small molecules, in metal-free hydrogenation or polymerisation processes.[1] While typically performed in solution, FLP chemistry in the solid state has been reported as well.[2]
Herein, we showcase how mechanochemistry can be explored in FLP chemistry enabling the formation of highly reactive solid-state FLPs through the application of mechanical energy in ball milling devices. The simultaneous grinding of the FLP entities increases the interaction interface between the Lewis acids and bases, even facilitating reactions with gases used in the milling device.



The mechanochemical synthesis takes place in specialised, gas-treatable ball-milling jars within a planetary ball mill,[3] which allow the *in-situ* formation of the Tris(pentafluorophenyl)borane/ Tricyclohexylphosphane - FLP and the activation of CO_2. Solid-state NMR spectroscopy is used to gain structural insights into the formed FLPs as well as their reaction products. In particular, ^{11}B MAS NMR and the information it provides on quadrupolar coupling are used to track CO_2 insertion. Distance measurements between the nuclear spins of the phosphorus Lewis base and the boron Lewis acid provide further information on the synthesised FLPs. The results are supplemented by solution-state NMR and IR spectra.
A comparison of the mechanochemical reaction with the corresponding reaction carried out in an autoclave highlights the strong increase in efficiency of the ball-milling approach.

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Talk:
24

What the Adsorption Isotherm Cannot Resolve: Solid-State NMR and Atomistic Modelling of Confined CO_2

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Solid CO_2 sorbents are developed largely on textural criteria, yet materials almost indistinguishable by them can behave differently. The metal–organic framework (MOF) CALF-20 has a lower surface area than zeolite SSZ-13 (540 against 688 $m^2\ g^{-1}$) and a zero-loading isosteric heat within 1.6 kJ mol^{-1}, yet its IAST CO_2/N_2 selectivity is nearly three times higher. What separates them is not texture but the identity and dynamics of the adsorbed species.

Both are difficult to determine: adsorbed CO_2 is dilute, chemisorbed carbamic acid, carbamate and bicarbonate resonate between 150 and 170 ppm, where they may overlap framework signals, and physisorbed CO_2 appears near 125 ppm irrespective of its motion. An isotherm reports the sum of these contributions as a single number. For a decade my group has separated them by ^{13}C, ^{15}N and ^{29}Si solid-state NMR of sorbents dosed with $^{13}CO_2$ at controlled pressure, interpreted with DFT, grand canonical Monte Carlo and molecular dynamics.

In this talk I will consider several classes of sorbent. In amine-grafted mesoporous silicas, quantitative multiple cross-polarisation with T_1 relaxometry quantified six coexisting species as a function of pressure, their summed isotherms reproducing the manometric capacity (0.81 against 0.85 mmol g^{-1}) [1–3]. In CALF-20, the ^{13}C chemical shift anisotropy increased from 80 to 130 ppm with loading, revealing an orientationally ordered phase templated by the pore wall's alternating electrostatic potential, to which N_2 is largely insensitive; in covalent organic frameworks (COFs) under humidity, multi-exponential T_1 analysis resolved three CO_2 populations displaced by water. In sodium poly(heptazine imide) [4], a crystalline carbon nitride, two-dimensional ^{13}C–^{1}H correlation separated a carbamic acid resonance at 161.9 ppm from framework signals and placed it at the bridging −NH− groups. Polysaccharide sorbents are little explored for CO_2 capture and almost unstudied by NMR, yet are far cheaper than MOFs or COFs and can match COF-999, the direct air capture benchmark [5]. In aminated cellulose nanofibril aerogels, dipolar- and J-coupling-based two-dimensional experiments distinguished covalent grafting from self-condensation and monomeric from polymerised silane, heteronuclear correlation placed the carbamic acid in a strong hydrogen bond to a ring hydroxyl or adjacent propylamine, a ^{13}C–^{13}C double-quantum correlation excluded dimers, and chemisorbed CO_2 from air at 400 ppm was observed at natural ^{13}C abundance [6].

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Talk:
25

Optically addressable spin systems in diamond and proteins for sensing and imaging

D. B. Bucher, Garching/G

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Optically addressable spins have attracted significant interest for their potential in quantum sensing technologies. In the first part of this talk, I will present our recent advances using nitrogen-vacancy (NV) centers in diamond chips for nuclear magnetic resonance (NMR) microscopy. NV-doped diamond platforms enable the transduction of local magnetic resonance signals into optical signals, which can be captured over a wide field using a camera. This novel approach eliminates the need for traditional k-space sampling with magnetic field gradients, as used in conventional MRI. I will discuss the current limitations of this novel microscopy technique and outline prospects for future developments. [1]
In the second part, I will highlight our latest research on optically addressable spins in proteins—specifically flavin-based cryptochrome proteins. Upon excitation, these proteins generate radical pairs that can be detected optically and manipulated through radio wave-controlled spin chemistry. We further show that this optical spin interface is tunable by the protein structure. I will explain how these systems differ from the well-established NV center and discuss their potential as genetically encoded quantum sensors for future applications. [2]

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Talk:
26

Dye Sensitized ^{1}H and ^{13}C solid-state NMR at High Magnetic Fields

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NMR spectroscopy is one of the most versatile techniques to study the atomistic structure and dynamics of complex systems in their native environment. Yet, the application of NMR in many fields is still impeded by its intrinsically low sensitivity.[1,2]
Optically induced hyperpolarization techniques are particularly suited to alleviate this issue, because they can in principle generate very high nuclear polarization levels. Among many proposed avenues for optically induced nuclear spin hyperpolarization in solids, photochemically induced dynamic nuclear polarization (photo-CIDNP) is attractive, as it can in theory generate polarization levels up to 100%, it only requires irradiation with light, and can be active at high magnetic fields.[3] While solid-state photo-CIDNP was initially observed on ^{13}C and ^{15}N in biological systems such as flavoproteins and bacterial reaction centers,[4,5] we recently demonstrated that photo-CIDNP can also be utilized to generate ^{1}H bulk hyperpolarization with enhancements up to $\varepsilon = 100$ at magnetic fields as high as 21.1 T and under magic angle spinning.[6,7] In our experiments, ^{1}H hyperpolarization was generated locally using small molecular donor-acceptor molecules (D-A) and distributed to the bulk via ^{1}H-^{1}H spin diffusion opening the perspective to take advantage of the same workflow today used in microwave driven MAS DNP.[2]
Building on these experiments, we extended existing theoretical photocycle descriptions and identified new design principles to improve the performance of D-A systems.[8] We will present experimental confirmation of these design principles by magnetic field dependent photo-CIDNP experiments. A combination of theory and experiment allowed us to identify a new D-A system with improved performance reaching ^{13}C enhancements of -4500 at 14 T corresponding to a nuclear polarization of 16 %.
We will also report our progress on ^{1}H bulk hyperpolarization, where we show that minor structural optimizations significantly improve the relay to the bulk, which led to the observation of $\varepsilon > 1000$ at a recycle delay of 20 s.

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Talk:
27

Site-specific distance measurements using heteronuclear cross-relaxation dynamics under MAS DNP

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Dynamic nuclear polarization (DNP) has routinely been used to enhance magic-angle spinning (MAS) NMR signals uniformly. In recent years, there has been an emerging interest in using DNP to also achieve site specific enhancement.[1] One such approach is the Specific Cross Relaxation Enhancement by Active Motions under DNP (SCREAM-DNP), which exploits the fast reorientation dynamics of methyl groups, even at low temperatures.[2,3] The scope of this application continues to broaden, particularly through the use of ring puckering dynamics besides methyl reorientation, and by combining it with techniques such as rotational resonance.[4,5,6]

Typically, the polarization buildup in SCREAM-DNP experiments is analyzed by fitting to mono- or biexponential models. However, because the underlying spin dynamics is minimally described by the Solomon equations, exponential models are not fully able to describe the observed behavior. To address this limitation, we present a fitting approach based directly on the Solomon equations, offering a more precise description of such systems, and, most importantly, an informative physical interpretation of the obtained rate constants based on different processes in the multi-spin system. Besides detailed insights into the polarization transfer dynamics of systems containing methyl groups, this new approach allows a quantitative determination of the cross-relaxation rate constant between the methyl protons and a target nucleus. Based on the knowledge of this quantity, we were able to calculate site-specific, short range, effective interatomic distances to several heteronuclei (^{13}C, ^{31}P, ^{77}Se) using the well-known hydrogen-carbon distance within the methyl group as reference.

Literature:

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Talk:
28

RASER as a sensor for chaos, synchrony and self-organized MRI

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In this lecture I will focus on the para-hydrogen driven RASER (Radiofrequency Amplification by Stimulated Emission of Radiation, [1]) as a suitable sensor for the exploration of synchrony and chaos in spin systems having a sufficiently high population inversion. First a brief introduction in to the universal one-mode XASER equations (X = Laser, MASER, RASER) will be given. Depending on the order parameters of the XASER model three distinct fields in science emerge, i.e. 1. LASER physics, 2. the extended Maxwell-Bloch equations (RASER) and 3. Chaos theory (Lorentz equations). Neither chaos nor synchrony can be observed in the one-mode RASER, but for two or more interacting modes the whole palette of non-linear phenomena including period doubling, synchrony and chaos become observable. I present first experimental results for a para-hydrogen pumped two-mode proton RASER, where above mentioned non-linear phenomena occur under appropriate conditions. [2] Finally, I will introduce the physics of RASER MRI, where in the presence of a magnetic field gradient and in the absence of radio-frequency irradiation a one-dimensional magnetic resonance image forms in a self-organized way. First experimental results for proton RASER images show phenomena like interference-, out-leaking effects and image artefacts which are predicted by the RASER MRI theory. [3]

Literature:

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Talk:
29

Kinetic asymmetry drives directionality in an ATP-binding cassette transporter

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ABC transporters are among the largest and most widespread protein superfamilies[1]. Their dysfunction is associated with numerous human diseases and contributes to multidrug resistance. ATP binding and hydrolysis at the nucleotide-binding domains (NBDs) are transmitted to the transmembrane domains (TMDs), which create a pathway for substrate permeation across the membrane[2]. Despite extensive structural and computational studies, the molecular determinants that define the transition barriers of the transport cycle, and how the measured kinetics arise from them, have remained unknown. Furthermore, the physical principles dictating how such systems achieve directionality remain poorly understood.

Here we addressed these questions using an integrated approach involving time-resolved pulsed dipolar ESR spectroscopy, unbiased molecular dynamics simulations, and non-Markovian rate theory. We identify two conserved ionic locks within the nucleotide-binding domains that govern transition barriers and energy transduction: an intra-subunit inward-facing (IF)-lock and an inter-subunit outward-facing (OF)-lock. Mg^{2+}-ATP acts as a molecular key that disrupts the IF-lock, driving the forward transition. Following ATP hydrolysis, release of the γ-phosphate, which, together with Mg^{2+}, forms the pivot of the OF-lock, initiates the reverse transition. Directionality arises from kinetic asymmetry, driven by an anticorrelated exchange of the rate-limiting step between the consensus nucleotide-binding site and the transmembrane domains during forward and reverse transitions, respectively. Conservation of these molecular locks reveals a universal blueprint for ATP-driven mechanical transduction across the ABC superfamily.

Literature:

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Talk:
30

How do binary liquids demix in mesopores? NMR and MD applied to silica pores from 4 to 50 nm

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Separation of bulk-immiscible liquids with different polarity is known to be reproduced in porous media on the macroscopic scale, as can be found in soils, rocks and building materials. In mesopores, phase separation may also occur for totally miscible liquids, such as for acetone and water, or not at all for ideal systems, such as acetone and THF. Understanding and quantifying the conditions that lead to demixing are relevant, for instance, for catalysis research and for biochemical topics such as transport through cell membranes.

Combinations of bulk-miscible polar and non-polar liquids were studied while saturating mesoporous media of different pore sizes. For the example of acetone and cyclohexane, a clear apparent phase separation was observed by NMR relaxometry [1] and MD simulations [2], where acetone is preferably located at the polar silica wall and severely slowed down in its short-time translational dynamics; equivalent long-time diffusometry results by NMR agree in the sense that acetone diffusivity is reduced up to 1000 times compared to intraporous cyclohexane in 4 nm porous glass. The difference between adsorbed and non-adsorbed phases is most striking in frequency-dependent T_1 relaxation where surface-mediated RMTD [3] and bulk-like isotropic reorientation are clearly distinguished for several systems, including water and acetone. The equivalence of ^{1}H and ^{2}H relaxation properties supports the RMTD model, i.e. purely intramolecular relaxation mechanisms. Investigations in controlled-pore glass (CPG) of up to 50 nm pore diameter confirm the apparently complete phase separation for acetone and cyclohexane which is further corroborated by freezing experiments of the same system, whereas mixtures of two non-polar liquids, depending on individual molecule-surface affinity, cover the range from ideal mixtures to noticeable concentration gradients that also affect freezing behavior of the confined mixtures.

The details of surface relaxation in silica and glass are investigated by deuteration of surface hydroxyl groups [4], or doping the surface with stable radicals. Strategies are presented to quantify the degree of demixing by means of computed radial density functions, MSD, neutron scattering as well as experimentally accessible relaxation and diffusion results.

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Talk:
31

^{57}Fe NMR is Great – No Irony

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Iron-57 is a spin ½ nucleus and the only NMR active iron isotope. Its low natural abundance (2.2 %) and extremely low gyromagnetic ratio (3.3 % relative to ^{1}H) make ^{57}Fe NMR spectroscopy challenging. The overall sensitivity is about three orders of magnitude smaller compared to ^{13}C at natural abundance. Despite these unfavourable magnetic properties, there is interest in ^{57}Fe NMR as it offers distinct advantages due to the high sensitivity of the nucleus to its chemical environment:[1] Like other transition metal nuclei, iron offers a very large chemical shift range covering several thousand ppm. With such a high signal dispersion, even minor structural changes result in separated ^{57}Fe signals, which allows for sensitive mapping of the electronic and magnetic surroundings of the iron atoms.[2] Secondly, while common NMR nuclei like hydrogen are often located at the periphery of transition metal complexes, the metal atom itself is associated with reactivity and therefore of special interest for direct probing. Given the inherent challenges in iron detection, ^{57}Fe NMR is still rather exotic. Currently, it is mostly applied for the investigation of Fe(0) and Fe(II) species, such as carbonyl complexes,[3] ferrocene derivatives[4] and iron in heme-like structures.[5]

Herein we present the solution state ^{57}Fe NMR analysis of diamagnetic tris(bipyridine)-iron(ii) and a series of related homoleptic iron complexes with substituted bipyridine ligands. To date only one representative of this substance class has had its ^{57}Fe chemical shift reported in the literature.[6] Utilizing both direct and indirect detection techniques, we analyse the influence of substituents and the substitution pattern on the central iron atom and its chemical shift. Our investigations extend the known range of ^{57}Fe shielding and establish a frame of reference for ^{57}Fe chemical shifts in iron bipyridine complexes. Furthermore, we demonstrate the power of ^{57}Fe NMR by the distinction of facial and meridional isomers, enabling the full signal assignment of these species in *fac/mer* mixtures.

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Talk:
32

Quantitative ESR-Based ROS Analysis: From Model Systems to Clinical Monitoring

Audrey Ayekoi, Max Fischer, Hicham Aissa, Benedict Munz, Andreas Günter, Tizian Boehmerle, Jan-Steffen Pooth, Sandra Jukic, Richard Schäfer, Stefan Weber, Friedhelm Beyersdorf, Erik Schleicher

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Quantifying reactive oxygen species (ROS) in biological systems requires highly sensitive and selective detection methods. Here, we present an approach based on electron spin resonance (ESR) spectroscopy that uses cyclic hydroxylamine spin probes to study the kinetics of ROS formation and deactivation.

First, we validated the ESR-based spin-counting strategy by examining the chemical selectivity and membrane permeability of the TMTH spin probe. Under the selected conditions, we demonstrated that TMTH exclusively reacts with superoxide. Subsequently, we applied this method to three different clinical scenarios. In one scenario, we monitored systemic ROS concentrations in patients undergoing coronary artery bypass surgery. We examined two different pumping techniques and the effect of vitamin C on ROS dynamics (1). Second, we quantified the long-term (49-day) accumulation of ROS in red blood cell concentrates and correlated it with hemoglobin oxidation state (2). Third, we performed a systematic analysis of components of a model circulatory system to identify sources of radical formation in extracorporeal medical devices, such as oxygenators.

Our results demonstrate that ESR spin probing is a robust, quantitative method for analyzing redox activity across scales, from medical device components to systemic clinical applications.

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Talk:
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How posttranslational modifications shape cell cycle checkpoint proteins – towards integrating structural biology and chemical biology toolsets

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Intrinsically disordered proteins (IDPs) and proteins containing intrinsically disordered regions (IDRs) are prominent in regulatory processes, such as cell cycle checkpoints. Since IDPs/IDRs are particularly accessible to posttranslational modifications, high compositional heterogeneity results, which allows them to act as integrative signalling hubs. This, however, also complicates their structural analysis. Preparation of samples with high fidelity to their cellular signalling state, in conjunction with a multi-methodological approach, is crucial for the detailed analysis of structural subtleties of these proteins.

The phosphatase Cdc25C is a major positive regulator of the G2-M cell cycle transition and phosphorylation within its IDR after DNA damage reduces Cdc25C cellular activity by retention in the cytosol. We investigate the interaction of Cdc25C-IDR with the scaffold protein 14-3-3 via multiple, previously uncharacterized phosphorylation sites. Utilizing synthetic and recombinant sample preparation together with NMR, ITC and MS measurements we determined binding strength and interaction sites of the complex. Besides the canonical pS216, two previously uncharacterized phosphorylation sites mediate binding at low micromolar-binding affinities. We are currently testing hypotheses on potential bivalent binding modes, stoichiometry and structure of the complex as well as implications for integration of different signalling pathways.

Additionally, to enable stable, site-specific phosphorylation states we work on the incorporation of non-hydrolysable phospho-tyrosine in recombinantly expressed proteins. We aim to develop an easy-to-use genetic code expansion kit for *E. coli*, using protein engineering to tackle bioavailability as well as inefficient incorporation.

Together, these directions pursued in the lab, aim to enable detailed mechanistic and structural characterization of phosphorylation-dependent regulation in intrinsically disordered regulatory proteins.

Talk:
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Detection of XH-pi Interactions in Intrinsically Disordered Proteins: A Combined NMR and MD/DFT Approach

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Non-covalent interactions (NCIs) play central roles in the structure, stability and dynamics of proteins and other biomolecules. A class of NCIs are unconventional XH-pi hydrogen bonds, in which XH and pi groups act as hydrogen bond donors and acceptors, respectively. Investigation of protein structure databases suggests that XH-pi interactions are prevalent in folded proteins, especially in their compact cores. Nevertheless, direct experimental evidence for their presence is limited to very few cases of CH-pi interactions in folded proteins. In intrinsically disordered proteins (IDPs), the lack of stable tertiary structure poses a challenge for structure-based prediction of XH-pi interactions. In this contribution, I will report on the NMR-based detection and verification of an NH-pi interaction in an IDP [1]. This interaction is observed between the NH of Gly22 and the aromatic ring of Phe20 in the E22G variant of Ab40 peptide linked to familial Alzheimer's disease. The presence of this interaction is suggested by several lines of experimental (NMR and Raman spectroscopy) and computational (MD/DFT) data and finally verified by detection of an ultraweak through-hydrogen-bond J coupling between the amide proton of Gly22 and all aromatic carbons of Phe20. I will also report on our latest results on a CH-pi interaction in another AD-related IDP. These are proof-of-principle examples of experimentally detected/verified XH-pi interactions in IDPs and pave the way for more thorough investigation of such interactions in IDPs, which seem to be more prevalent than is usually assumed.

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Talk:
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NMR-Guided Discovery of Membrane-Active Antiviral and Antimicrobial Peptides

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Membrane fusion between SARS-CoV-2 and host cells is mediated by the spike protein and involves the membrane-proximal external region (MPER), a tryptophan-rich sequence implicated in viral entry. We investigated the feasibility of MPER-derived peptides as potential antiviral agents and examined the structural determinants underlying their activity. A series of truncated MPER peptides was synthesised and evaluated for antiviral activity against SARS-CoV-2 in cellular assays, revealing potent inhibitory activity against different variants, with nanomolar IC_{50} values associated with sequences rich in aromatic residues. Using NMR spectroscopy, we demonstrate that these peptides adopt a stable α-helical conformation in solution and in membrane-mimetic environments, stabilised by intramolecular aromatic π–π stacking interactions among tryptophan and tyrosine side chains. Structure–activity analysis indicates that this aromatic network promotes α-helix stabilisation, mimicking the MPER structure of the post-fusion spike, and correlates with enhanced antiviral potency. Our findings reveal a structural mechanism by which aromatic stacking stabilises MPER helicity and drives antiviral activity, providing insights into peptide-based inhibition of viral membrane fusion and offering a framework for the rational design of SARS-CoV-2 entry inhibitors.

In the search for new antibiotics, we further uncover the mode of action of the recently identified bactericidal protein Ave1. Using NMR, we solved its three-dimensional structure, revealing a six-stranded β-barrel fold, and show that Ave1 disrupts microbial membranes. Furthermore, we demonstrate that synthetic peptides corresponding to positively charged regions of Ave1 exhibit antimicrobial activity. By characterising the interaction of Ave1 with lipoteichoic acid, a major component of the Gram-positive cell wall, our findings support a model in which Ave1 associates with the bacterial surface, from where it perturbs the plasma membrane, ultimately leading to membrane dissipation and cell death. This opens new routes for the development of novel antimicrobial peptides based on Ave1.

Talk:
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Solid-State NMR Spectroscopy Methods to Study Lipid Membranes

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Exploring the microscopic properties of lipid membrane models is important in a wide range of fields, including drug delivery and molecular biology. Solid-state NMR spectroscopy is arguably one of the most powerful methodologies for this purpose, enabling structural and dynamical information to be obtained at atomic resolution, even from samples containing isotopes at natural abundance.

In this presentation, I will describe the NMR strategy that we have been implementing in this context, based on proton-detected local-field and relaxation experiments combined with molecular dynamics simulations. Results from two of our ongoing projects will then be presented as examples: the study of how superchaotropic particles affect lipid membranes and the molecular modelling of myelin membranes.

Talk:
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From Molecular Interactions to Material Performance: Understanding Porous Materials

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The development of sustainable porous materials for CO_2 capture and separation requires a molecular-level understanding of how synthesis and structure influence surface chemistry, gas-solid interactions, and material performance. Magnetic resonance techniques offer valuable insights into these relationships, supporting the rational design of advanced materials for environmental applications.
Strategies for enhancing magnetic resonance sensitivity, including spin labels and isotopic labelling, will be discussed in the context of their application to porous materials and their synthesis. Examples will include the use of EPR to probe paramagnetic species and reaction processes in organosilica-based materials [1], alongside solid-state NMR to elucidate chemical environments and gas–surface interactions in carbon-based adsorbents. Particular emphasis will be placed on the molecular mechanisms governing CO_2 adsorption and the influence of surface functionalities and pore environments on adsorption performance. The integration of magnetic resonance with complementary techniques, including XPS, electron microscopy, and gas adsorption, provides a comprehensive approach to establishing structure–property relationships [2]. The discussion will conclude by highlighting current challenges and open questions in the molecular-level characterization of complex porous materials.

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Acknowledgements:
This work was developed within the scope of the project CICECO-Aveiro Institute of Materials, UID/50011/2025 (DOI 10.54499/UID/50011/2025) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020) & UID/PRR/50011/2025 (DOI 10.54499/UID/PRR/50011/2025), financed by national funds through the FCT/MCTES (PIDDAC). It has received funding from the European Research Council under the European Union's Horizon Europe research and innovation program (GA 865974) and by FEDER - Fundo Europeu de Desenvolvimento Regional funds through the Programa Inovação e Transição Digital (COMPETE 2030) and by Portuguese funds through FCT- Fundação para a Ciência e a Tecnologia in the framework of the project COMPETE2030-FEDER-00776600 (CharM). FCT is acknowledged by MAOL for a Junior & Assistant Researcher Positions (CEECIND/01158/2021 & CEECIND/08302/2024). NG and MAOL acknowledge funding from the European Union's Horizon 2020 research and innovation programme No. 101065059 and 101090287, respectively.

Talk:
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Advanced NMR Spectroscopy for Electrolysis Applications: An Overview

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NMR techniques are established and versatile analytical methods in many scientific fields, such as organic and material chemistry or medical diagnostics. In electrochemistry, however, application of NMR spectroscopy has been limited due to challenges caused by the interactions of the involved magnetic fields and conductive components inherent to materials and reactions in this field. Nonetheless, battery and electrolysis research significantly benefits from insights enabled by magnetic resonance techniques, and thus developments have been spearheaded by several NMR research groups either obviating these challenges, minimizing their impact, or even exploiting them for benefit.

This contribution outlines some of our efforts to establish NMR spectroscopy for the investigation of electrolysis reactions and materials, granting novel and unique insights. E*x situ* NMR was utilized for the study of ionomer materials, specifically proton exchange membranes (PEMs). Solid state NMR and relaxation studies offered correlated insights into the evaluation of accelerated testing protocols for PEM degradation by revealing shortcomings compared to the actual deterioration of PEMs in electrolyzer operation [1]. While NMR investigations of accelerated PEM degradation have been conducted previously, this work highlights the merits of supporting magnetic resonance techniques with cross-scale analytics that facilitated the construction of a mechanistic picture with combined chemical and structural degradation pathways.

Furthermore, benchtop NMR techniques are highlighted as a valuable tool for ionomer analysis in an industrial setting [2]. While detailed analysis of changes in ionomer chemistry is only feasible by high-field magic angle spinning (MAS) NMR, a structure-property relationship can be constructed utilizing pulsed field gradient (PFG) NMR methods available at benchtop class spectrometers. Thus, routine quality control as well as studies on ionomer chemistry and properties can be reliably and quickly conducted in applied settings without the need for complex electrochemical cell testing.

Finally, first insights into a novel technique combining NMR, numerical quantum-mechanical optimizations, and finite element simulations are presented [3]. This approach utilizes quantum optimum control (QOC) to exploit magnetic field distortions induced by metallic electrodes as predicted by simulation, enabling B_0 and B_1 sensitive NMR investigations aimed at electrode surfaces or volumes enclosed by battery electrodes.

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Talk:
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Revealing Ion Exchange and Transport Pathways in Hierarchical Porous Carbon Electrodes

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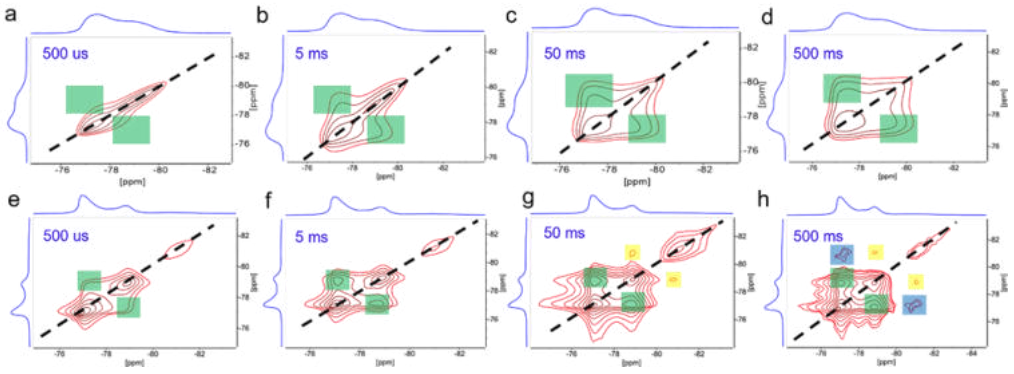
Ion transport within porous carbon electrodes strongly influences the performance of electrochemical capacitors, yet exchange dynamics across heterogeneous pore networks remain difficult to quantify. Here, we present a quantitative framework for extracting ion exchange kinetics from two-dimensional exchange spectroscopy (2D EXSY) NMR that accounts for asymmetric ion populations and relaxation effects. The method employs a lognormal distribution of exchange rates to capture the intrinsic heterogeneity of ion motion in porous materials. Applied to aqueous LiTFSI electrolyte confined in mesoporous CMK-3 and hierarchical ST-CMK-3 carbons, the approach resolves multiple ion-exchange pathways spanning ex-pore, mesopore, and micropore environments. We report the first observation of three-site ion exchange in porous carbon electrodes and show that ion mobility and effective diffusion are enhanced in the hierarchical ST-CMK-3 porous carbon [1]. Additionally, PFG NMR studies support the observation of enhanced transverse diffusivity across the interconnected mesopore structure of ST-CMK-3, relative to the archetypal CMK-3 carbon. These results establish quantitative links between pore architecture and ion-transport efficiency, providing insights for the design of high-rate carbon electrodes for next generation electrochemical capacitors.



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Talk:
40

Solid-state NMR spectroscopy for catalysis: New concepts for self-assembling Supported Ionic Liquid Phase catalysts and heterogeneous photocatalysis in real time

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Many large industrial processes are driven by heterogeneous catalysts. They are stable, easy to separate and reuse, but often lack the well-defined active sites that make homogeneous catalysts selective. Solid-state NMR spectroscopy under Magic Angle Spinning (MAS) allows to obtain molecular-level information about heterogeneous catalysts, to resolve surface species, dynamics and host-guest interactions. It is thus key for the knowledge-driven design of better catalysts.

An emerging concept for a new class of catalysts are Supported Ionic Liquid Phase (SILP) catalysts: In SILPs, a thin film of an ionic liquid (IL) film containing a molecular catalytic complex is deposited onto a solid support, thus combining advantages of both homogeneous and heterogeneous catalysis. However, the position of the catalytic complex in the film is so far little controlled. We have recently introduced a series of four tailor-made ionic liquids. By MAS NMR, we show how these ILs self-assemble on a porous silica support as ordered monolayers.[1] Used as ligands, the ILs also direct a catalytically active metal complex into a well-defined distance from the support. This strategy allows for the immobilization of a molecular Pt(II) catalyst on silica.[2]

A particular challenge for solid-state NMR is the real-time observation of heterogeneous photocatalysis. We have recently reported operando MAS NMR observation of photoreforming of ^{13}C-labelled methanol by light irradiation of a transparent sapphire rotor.[3] Meso- and macroporous, rotor-sized silica monoliths serve as catalyst support, titania (anatase) as photocatalyst. The large pore volume of the monoliths accommodates the liquid substrate, while pores wider than the wavelength of visible light enhance light penetration and catalytic activity.[3] This approach opens a pathway for operando investigations of heterogeneous catalysis by MAS NMR.

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Talk:
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EPR Characterization of Radical Dendrimers for Metal-Free MRI Contrast Agents

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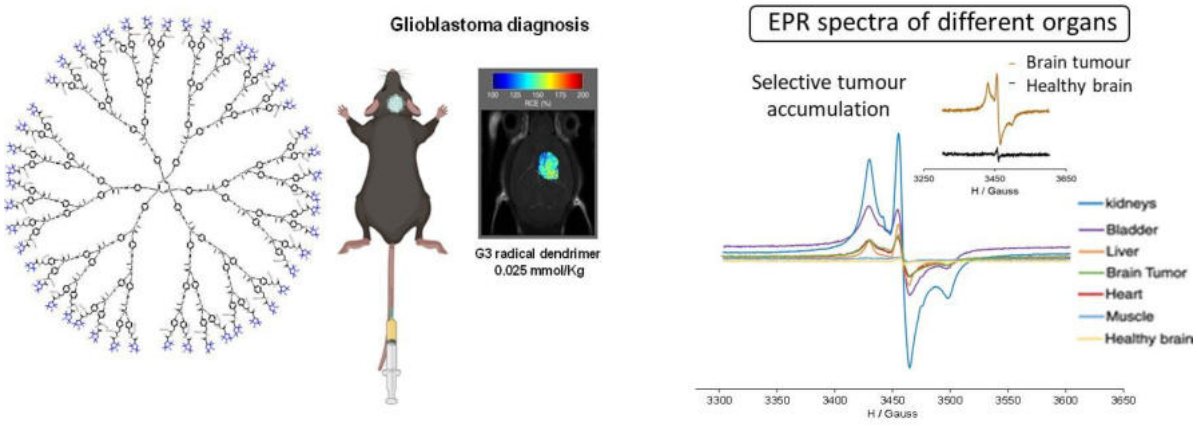
Gd(III)-based chelates are the most widely used contrast agents (CAs) in clinical magnetic resonance imaging (MRI). However, alternatives to such metal-based CAs are highly required to overcome their established toxicity.
Stable organic radicals are promising T_1 contrast agents, providing paramagnetic properties without the need for toxic metals. In particular, conjugating multiple radicals to dendrimeric macromolecules (radical dendrimers) enhances their contrast and stability compared with isolated radicals. We synthesized and characterized different families of water-soluble radical dendrimers that provide strong contrast enhancement in both *in vitro* and *in vivo* studies.[1]
EPR spectroscopy served to characterize these species, showing that radical units in higher-generation dendrimers exhibit reduced mobility and stronger local spin exchange. In addition, EPR combined with molecular dynamics simulations revealed that radical location, water accessibility, and hydrogen-bonding interactions with nitroxide groups are key determinants of relaxivity.



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Talk:
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Probing Cu^{2+} Dopant Sites in Zn-based MOF-74 via EPR Spectroscopy

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Metal-organic frameworks (MOFs) continue to attract significant attention due to their tunable pore structures, chemical versatility, and potential applications in gas storage, catalysis, and separations. [1, 2, 3, 4] Among these, MOF-74 (also known as CPO-27) is a widely studied framework for the study of hydrogen isotope separation and storage because of the presence of open metal sites. [5, 6] Introducing paramagnetic dopants like Cu^{2+} in MOF-74 (Zn) facilitates the utilization of electron paramagnetic resonance spectroscopy (EPR), which is very sensitive to the local environment of the probe.

We investigated Cu^{2+}-doped MOF-74 (Zn), using EPR to study the structural properties of the framework for utilization in the field of hydrogen isotope storage and separation. Upon measuring with continuous wave EPR, it is evident from the EPR parameters that the Cu^{2+} species are incorporated in a distorted octahedral environment. Treating the as-synthesized sample with pulsed EPR techniques like 2pESEEM, 3pESEEM, and HYSCORE spectroscopy reveals further details about how the Cu^{2+} species is incorporated into the framework. It is evident that the Cu^{2+} species is binding to five oxygens from the framework and one solvent molecule. Upon activation, the solvent molecule gets removed, and the local environment of the Cu^{2+} species changes. Such an open metal site is crucial for hydrogen isotope applications. Further, studies with EPR will reveal the host-guest interaction of the framework and the hydrogen gas molecules.

This work is supported by DFG Project (ID 443871192), GRK 2721: "Hydrogen Isotopes 1,2,3 H".

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Talk:
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Relaxation enhancement and electronic structure investigations in transition metal (Cu, Ni, Fe) doped carbon nitride materials

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Due to the warming of the planet from greenhouse gas emissions, graphitic carbon nitride materials have been extensively studied given their unique ability to generate value-added hydrocarbons from the reduction of CO_2; albeit with relatively low efficiencies compared to other photocatalysts [1]. The popularity and ease of synthesis of carbon nitride materials have led to a multitude of studies that have demonstrated their usefulness in a variety of different photochemical reactions; and, in many cases their catalytic output has been drastically increased by the incorporation of transition metal ions either by direct chemical modification or via metal-doping and impregnation schemes [2]. While the catalytic output is often increased substantially, the underlying mechanisms for these increases are often highly variable due to the myriad of starting materials, synthesis conditions, resulting morphologies, and doping schemes thereby necessitating further studies into the electronic coupling of the photocatalytic π-delocalization cloud to the transition metal dopants. To this end, we herein present an investigation into the modifications in electronic structure induced by the wet-impregnation of transition metal ions (Cu, Ni, and Fe) into the graphitic carbon nitride framework. Using a combination of XAS, EPR spectroscopy, and SQUID magnetometry methods, we present a correlation between the shift in effective g-value observed in the transition metal dopants and an enhancement in electronic relaxation rate in the photocatalyst core structure; thereby elucidating a cooperative behavior behind one of the likely many contributors to what is typically referred to as synergy between transition metal dopants and graphitic carbon nitride photocatalysts. Given the recent interest in spin-dependence in photocatalyst materials [3], these findings suggest a potentially viable avenue for similar spin-dependent photocatalytic modulation in metal-doped graphitic carbon nitride materials.

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Talk:
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Development of EPR and ENDOR analysis methods

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EPR and ENDOR spectroscopy are methods of choice to identify structural information on molecular systems by detecting the interaction of an electron spin with its magnetic environment. ENDOR specifically detects the interaction of an electron spin with a nearby nuclear spin. After performing the experiment, the structural information is usually derived by data analysis methods, which depend on both the applied methods and the desired information.

Usually, experimental ENDOR spectra are compared to simulated spectra. Thus, the derived information is limited to the representation of the experiment by the simulation. Advances in experimental setup constantly increase the resolution of spectra, e.g. by enabling measurements at higher magnetic fields, with higher pulse power or with shaped pulses. This increases the information content of the spectra and more sophisticated and detailed simulations are required, especially when the effect of pulse sequences can no longer be approximated by a line shape function. A suitable method to directly identify these effects are simulations of the spin dynamics.
Here, the development and the applications of a spin dynamics simulation routine for ENDOR spectroscopy are described. As an example, the analysis of ^{19}F-ENDOR spectra is demonstrated, where, depending on the experimental setup and the sample, it can be required to include effects of power broadening, the chemical shielding anisotropy or nuclear dipolar couplings in the simulations. [1-3]

Suitable data analysis also enables the extraction of additional information that was so far hidden in experimental data. 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. 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. [4,5] 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. [6] In the second part of the contribution, it will be shown how the dependence on θ_2 can be used to identify local spin concentrations.

Literature:

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Talk:
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High and Selective Ion Conduction in Electrolyte-Host Materials – Investigating Confinement Effects using NMR Crystallography

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Porous materials offer potential for applications as diverse as gas storage and separation, catalysis, electronic and ionic transport, and sensor design. A significant advantage of this material class is that adapting pore sizes and interconnectivities, as well as the chemical composition of the inner surfaces, provides a unique and flexible handle to influence the properties of an adsorbed fluid guest phase. For example, porous materials are considered as hosts for electrolytes in separators of electrochemical energy storage and conversion devices, where high ionic conductivity should be paired with selective transport [1]. The spatial and chemical constraints of the structured hosts impose a shape on the adsorbed fluid electrolyte phases and enforce interactions at the guest-host interfaces. If the dimension of the constraints reaches the nanometre scale, confinement effects on properties like mass and charge transport emerge. Recent results suggest that the complex interplay between confinement-induced guest-host interactions and the mobility of mass and charge carriers can lead to exceptional properties in guest-host materials [2].
The lecture will demonstrate, using mainly two examples, how 2D and 3D nanoscale confinements alter the ion transport of embedded aqueous electrolyte phases. Using a series of lithium-ion-exchanged layered silicates [3], we investigate the trend of lithium-ion mobility and transport as a function of interlayer distance and water content. The second example focuses on sulfonated aromatic frameworks that exhibit outstanding proton conductivities of up to 2 Scm^{-1} when saturated with water, despite having pore spaces in the smaller micropore region [2]. Both studies employ an integrated approach that combines X-ray scattering, multi-nuclear solid-state NMR spectroscopy, NMR diffusometry, electrochemical impedance spectroscopy, and molecular dynamics simulations. In this way, we derive the structural details at the interfaces and obtain information about the interactions between the electrolyte and the host. Additionally, the studies provide insight into the local dynamics and the long-range transport. The derived transport mechanisms demonstrate how these properties are related to ionic conductivity in systems where the counterions are immobilized on the host frameworks.

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Solid-state ^{13}C and ^{15}N NMR of Functional Organic Materials

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Solid-state ^{13}C and ^{15}N NMR, ideally with spectral editing, is the best available method for characterizing the structure of insoluble organic materials. Nevertheless, due to distorted peak intensities in simple CP spectra, peak splittings from packing effects, and wishful thinking, routine ^{13}C ssNMR spectra of insoluble materials are sometimes misinterpreted. Two examples will be discussed in this talk. Based on chemical-shift analysis in quantitative multiCP ^{13}C spectra and in multiCP ^{15}N spectra, we show that a promising "COF" (covalent organic framework) is not a framework at all. Secondly, in an amine-substituted tricyclic electrode material used in lithium-ion batteries, quantitative direct-polarization (DP) ^{13}C and ^{15}N spectra with ^{1}H dipolar dephasing show that two central nitrogen atoms are not bonded to hydrogen, invalidating the structure presented in several high-profile publications. Fast, nonexponential ^{13}C and ^{15}N spin-lattice relaxation likely due to unpaired electrons made DP the best choice for quantitative NMR. Peak splittings are shown to be due to symmetry-breaking hydrogen bonding, using a simple precursor as a model system. [1]

In biodegradable, easily accessible polyethylene-like polyesters made from *N*-carbon diacids (*N* between 11 and 48) with $^{13}C_2$-ethylene glycol, NMR can characterize the crystalline chain conformation through tensor correlation and the crystallite thickness through ^{1}H spin diffusion with ^{13}C detection. CODEX ^{13}C NMR is well suited for distinguishing *anti* and *gauche* conformers of the $O^{13}C$-^{13}CO segments. NMR reveals several types of oxygen-induced *gauche* conformers in the crystallites and at the interface with the amorphous layers. For long diacids, the diesters exclusively form interfacial layers, so *N* controls the crystallite thickness. [2] While the polyesters with odd *N* are all-*anti* like polyethylene, those with even *N*, including the important PE-2,18 material, contain double kinks (*gauche*$^+$/*anti*/*gauche*$^-$) in their crystalline diol segments, as deduced from static 2D NMR and quantum-chemical calculations of the $O^{13}CH_2$ chemical-shift tensors. Dynamic *gauche*$^+$/*gauche*$^-$ disorder and the associated stabilizing increase in the entropy of the crystallites raises the melting point of PE-2,18 by ~10 K.

The talk will conclude with a brief review of Fermi's Golden Rule (FGR) in quantum dynamics: when it fails and when it works. FGR, claiming linear $P_{i\to f} = W\,t$, often represents invalid solutions of the Schrödinger equation under a sinusoidal perturbation, while the nonlinear Rabi oscillations familiar in magnetic resonance apply far beyond two-level systems.

Literature:

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Talk:
47

Mapping the Weak Structure of Disordered Loops in proteins using DEER-Restrained Ensemble Modelling

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Intrinsically disordered regions are increasingly recognized as functionally essential elements in proteins, yet they remain largely inaccessible to standard structural biology, which is built to resolve order, not disorder. Characterizing their "weak structure" — the biased, non-random conformational preferences that disordered segments can retain despite lacking a defined fold — calls for methods that can extract quantitative structural restraints directly in solution and integrate them into ensemble descriptions, rather than single static models. The combination of site-directed spin labeling and DEER are naturally suited to this problem, but turning a handful of distance distributions into a trustworthy structural ensemble is not automatic.

In this talk, we will use the C-terminal loop of human Apoptosis-Inducing Factor (AIF) as a working example of this approach. This ~40-residue loop is disordered in the available crystal structures and undergoes a redox-linked order/disorder transition that is central to AIF's dual role in mitochondrial respiration and apoptosis. Combining homodimer and orthogonal (nitroxide/Gd^{3+}) spin labelling, we obtained restraints to generate and refine conformer ensembles with MMMx. The resulting structural picture is a loop that samples a broad conformational space while showing a weak preference for the inter-monomer cleft. The methodological side of the analysis will be shown emphasizing how to test the robustness and reproducibility of the fitting procedure, how to distinguish genuine conformational bias from fitting artefacts, and how ensemble-refined models compare against MD-derived and fully random references.

Talk:
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New solid-state NMR approaches to decipher the molecular organization of fungal and yeast cell wall

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Most microbes possess a "cell surface", i.e. a critical surface architecture which can have several purposes: protection against the external environment, a mimicry strategy to evade host defenses, or a pathogenic molecular weapon to damage host cell membranes. Molecular understanding of the microbial cell envelope remains one of the most active research fields in microbiology, because many essential processes related to the survival of the microbe and its ability to infect host cells are taking place at the cell surface and are driven by surface components. The ability to study such cell surfaces at a molecular level is of prime interest, to understand how pathogenic and parasitic microbes can survive, proliferate and carry out their harmful action. Current state-of-the-art analytical approaches to study cell surface have two main drawbacks: (i) they are destructive or rely on the extraction of weakly-bound molecules, requiring chemical or biochemical methods prior to the analysis. (ii) Because each component is quantified in isolation, the global organization and interplay between components is missing. Here we present our recent advances using solid-state NMR spectroscopy to investigate the molecular organization of fungal, bacterial and yeast cell surface at atomic resolution: the architecture of Aspergillus fumigatus cell wall during its conidial morphotype transition (1), the molecular distinction between cell wall and capsular polysaccharides in Cryptococcus neoformans (2) and new NMR approaches to determine polysaccharide configuration in cellulo (3)

(1) Solid-state NMR molecular snapshots of Aspergillus fumigatus cell wall architecture during a conidial morphotype transition.
Lamon G, Lends A, Valsecchi I, Wong SSW, Duprès V, Lafont F, Tolchard J, Schmitt C, Mallet A, Grélard A, Morvan E, Dufourc EJ, Habenstein B, Guijarro JI, Aimanianda V, Loquet A.
PNAS 2023
(2) Molecular Distinction of Cell Wall and Capsular Polysaccharides in Encapsulated Pathogens by In Situ Magic-Angle Spinning NMR Techniques.
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(3) On-Cell Detection of Polysaccharide One-Bond 1JCH Couplings by Proton-Detected Solid-State NMR.
Lends A, Lamon G, Vallet A, Grélard A, Morvan E, Aimanianda V, Schanda P, Loquet A.
J Am Chem Soc. 2026

Talk:
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Combining solid-state NMR with surface and imaging techniques to unravel melittin–membrane interactions

I. Marín-Montesinos, Aveiro/PT, A. Chacón Calderón, Aveiro/PT, P. Zelenovskii, Aveiro/PT, M. Soares, Aveiro/PT, E. C. Wrobel, São Carlos/BR, O. N. Oliveira Jr., São Carlos/BR, D. Pereira, Aveiro/PT, M. Sardo, Aveiro/PT, L. Mafra, Aveiro/PT, A. Barros-Timmons, Aveiro/PT

Dr. Ildefonso Marín-Montesinos, Department of Chemistry & CICECO – Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal

Melittin, the main component of bee venom, is one of the most studied antimicrobial peptides, yet there is still no agreement on how it breaks a membrane: depending on conditions it has been described as forming pores or as acting more like a detergent. Much of this uncertainty comes from studies that relied on a single technique. Here we take a multidisciplinary approach, combining methods that each probe a different length scale, to build one coherent picture of the interaction. Using a two-lipid membrane that mimics the inner membrane of *Escherichia coli* (DOPE:DPPG 4:1) at two loadings (lipid-to-peptide 30:1 and 10:1), we brought together Langmuir monolayers with BAM and PM-IRRAS at the air–water interface, atomic force microscopy on thin films, solid-state NMR (^{1}H, ^{13}C, ^{31}P) on lipid bilayers, and molecular dynamics simulations.

Cross-checking these complementary methods shows that melittin acts in a concentration-dependent way. At low loading it stays mostly at the surface, causing a small area expansion and only mild, asymmetric lipid reordering, in line with a carpet-like mechanism. At higher loading the membrane takes up more water, the chains become more disordered, the bilayer thins, and its shape is remodelled, pointing to transient pore formation. Solid-state NMR was central to resolving the headgroup and chain dynamics, while the interfacial, microscopic and computational data placed these atomic-level changes in their wider context; across every technique the anionic lipid DPPG was more strongly affected than DOPE [1]. Integrating these approaches overcomes the limits of any single method and provides a robust framework that can be extended to other peptides and membrane systems.

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Talk:
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Integrated Solid-State-to-Solution NMR Assignment and Solvent Accessibility Mapping of Tryptophan Synthase

D. Blokhin, Dortmund/DE, H. Aucharova, Dortmund/DE, A. Klein, Dortmund/DE, S. Vasa, Dortmund/DE, R. Linser, Dortmund/DE,

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Tryptophan synthase (TS) is a 144 kDa αββα heterotetrameric enzyme complex that catalyzes the final step of L-tryptophan biosynthesis by coupling reactions in the α and β subunits. Its catalytic cycle involves long-range allosteric communication, ligand-dependent conformational changes and intermediate channeling through the inter-subunit tunnel. These properties make TS an important target for residue-resolved studies in solution. However, its size, spectral overlap and rapid relaxation strongly limit conventional solution NMR assignment strategies.

Here, we present an integrated assignment workflow combining protein expression in uniformly $^{2}H/^{13}C/^{15}N$-labeled ISOGRO medium, high-dimensional MAS solid-state NMR, automated computational assignment and transfer to solution NMR spectra. The use of perdeuterated, $^{15}N/^{13}C$-labeled amino acid mixtures from ISOGRO, obtained from algae for bacterial growth in H_2O instead of a glucose-based minimal medium, achieves a high level of amide protonation while maintaining a high level of deuteration in the side chains and hence grants narrow protein resonance lines [1]. As additional samples, three independently expressed TS samples were prepared by supplementing the medium with unlabeled Leu, Val or Glu. Comparison of the uniformly ISOGRO-labeled TS sample with these amino-acid-unlabeled preparations provided residue-type information.

To accelerate the assignment process, we developed an auto-assignment script that integrates complementary restraints from experimental chemical shifts, chemical-shift predictions, subunit belonging and residue typing. Together, these restraints enabled globally consistent residue-to-spin-system assignment of TS in the solid state.

The resulting solid-state assignments were subsequently transferred to solution NMR spectra using a dedicated solid-to-solution matching procedure. This transfer assignment enabled interpretation of the limited set of solution-state TS spectra. The assignments obtained owing to this two-step approach allowed downstream NMR characterization of TS in solution, exemplified via analysis of solvent accessibility combining SEA-TROSY [2], CLEANEX and solvent-PRE experiments. These data identify surface-exposed and protected amide sites and provide residue-specific information on solvent interaction, exchange behavior and structurally shielded regions of TS under monomeric conditions in solution.

Our integrated strategy demonstrates that ISOGRO-based uniform $^{2}H/^{13}C/^{15}N$ labeling, MAS solid-state NMR, automated assignment with complementary restraints and solid-to-solution transfer can serve as a practical route towards insights for large protein complexes that are challenging for conventional solution NMR.

Literature:
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Talk:
51

Aggregation kinetics and amyloid fibril structure probed by solution and MAS solid-state NMR spectroscopy

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Abstract

Systemic antibody light chains (AL) amyloidosis is characterized by deposition of amyloid fibrils derived from a particular antibody light chain. It has been shown that soluble oligomeric protein has a direct cytotoxic effect on cardiomyocytes prior to protein aggregation and organ malfunction. Removal of circulating pathogenic light chains by chemotherapy yields a drastic reduction of the concentration of biomarkers reporting on cardiac dysfunction.

We have used solution and MAS solid-state NMR to characterize the aggregation of a particular patient protein. The focus is put on a human protein sequence for which adipose and heart tissue material is available from a patient. It is shown that *ex vivo* material allows to reproduce the amyloid fibril structure *in vitro* by employing a seeding procedure. MAS solid-state NMR experiments yield information on the conformation of the amyloidogenic core and allow to probe interactions with small molecules that potentially interfere with the aggregation process. Using solution-state NMR spectroscopy, we follow the individual steps involved in protein misfolding at atomic resolution. We show that the natively folded protein first partially unfolds, before it converts into a high molecular weight molten globule like structure. Oligomer formation implies high local concentrations of aggregation prone regions which catalyze the subsequent conversion into amyloid fibrils. We show that the topology of the aggregated state is determined by balanced electrostatic interactions in the core of the fibril, resulting in an anti-parallel arrangement of the beta-sheets around the conserved disulfide bond.

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Talk:
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In-situ and Operando ESR in Heterogeneous Gas Phase Catalysis

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The properties of many heterogeneous catalysts depend crucially on their environment (temperature, pressure, gas-phase composition, etc.), making characterization under catalytically relevant conditions important for a mechanistic understanding of these systems. Changes induced by the environment can encompass structural and electronic properties, making an atomic-level characterization challenging. In recent years, a range of techniques, including ESR spectroscopy have been developed to investigate catalytic systems under in situ/operando conditions. While ESR spectroscopy has been shown to provide important insight into the aforementioned questions, it is important to emphasize that no single method provides a comprehensive picture. Thus, a combination of different techniques is necessary.
In this contribution, we will focus on heterogeneous gas-phase catalysis. While paramagnetic species are the primary target of most ESR spectroscopic studies in catalysis research, this discussion will also demonstrate how characterizing collective magnetic properties, such as ferromagnetic phases, can provide insights beyond those of standard characterization techniques. Gas-phase catalysis is usually performed continuously, allowing the reactant to flow through a catalyst bed. This implies that the gas-phase composition changes along the reactor bed. Consequently, it is expected that the catalyst's properties will change. Iso-potential spectroscopy, which uses a profile reactor setup, provides an opportunity to characterize these changes. In this presentation, we will discuss recent results from an exploratory study of a V/TiO_2 catalyst used for the de-NO_x reaction, i.e., the comproportionation of NO with ammonia in the presence of oxygen.

Talk:
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EPR investigations of Molecular Heterogeneous Catalysis in Confined Geometries

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Molecular heterogeneous catalysis in mesoporous systems combines the advantages of homo- and heterogeneous catalysis. On the one hand, the catalyst that is immobilized in the mesopore by means of a linker, is molecularly well defined, enabling microscopic understanding of reaction mechanisms. On the other hand, immobilization allows facile separation of catalyst and product. Furthermore, the confined geometry of the mesopore can improve selectivities and productivities of the catalytical reactions.[1]

Here we present our investigations of cobalt(II)- and copper(II)-catalyzed reaction with the focus on magnetometric and electron paramagnetic resonance techniques. In direct catalytic asymmetric 1,3-dipolar cycloadditions with cobalt(II)-based polyfunctional Lewis acid / azolium – aryloxide catalysts, our measurements revealed the high-spin state of the catalyst.[2] Interestingly, recently we have contributed to a study on copper-catalyzed asymmetric Michael additions, where greatly enhanced yields and enantiomeric excesses were found in mesoporous silica compared to the same catalyst under homogeneous conditions. EPR proved that the catalyst is homogeneously distributed in the mesopores. In addition, EPR revealed that interaction with the substrate traps part of the catalyst into an unproductive state in homogeneous conditions but not in mesoporous systems.

Literature:

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Talk:
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Paramagnetically Doped Metal–Organic Frameworks for Dynamic Nuclear Polarization: An EPR Study

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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: ZIF-8, which is a zinc-based zeolitic imidazolate framework, and to investigate its gas adsorption behavior. To gain insight into the local environment of the ZIF-8 framework and the host–guest interactions occurring during gas adsorption, high-spin paramagnetic metal ion like Mn^{2+} ($S=5/2$) was introduced as spin probes into the frameworks. Such S-state ions (with minimal orbital angular momentum) are likewise 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 in MOFs 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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Talk:
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Determination of an unusual positive Cu hyperfine coupling in a square-planar copper(II) complex using multi-frequency EPR and W-band TRIPLE spectroscopy

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

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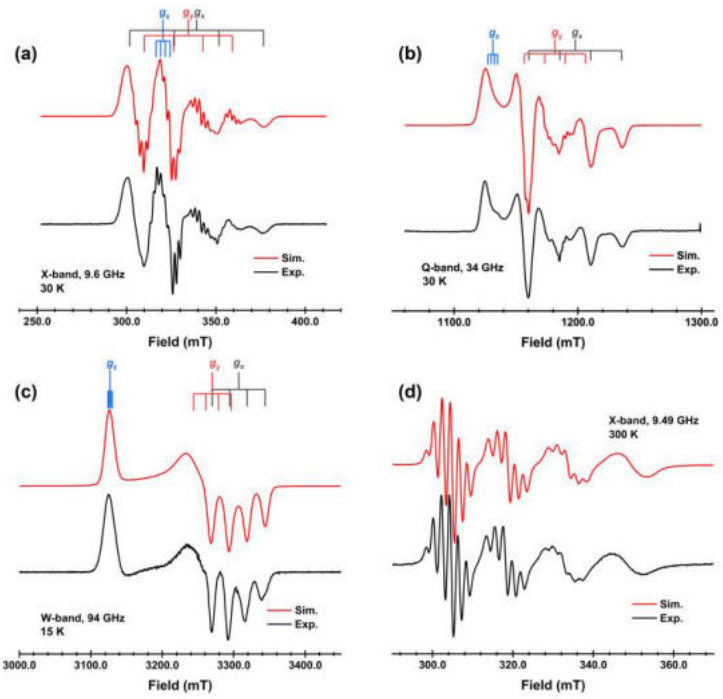
Copper(II) sites are crucial cofactors in enzymes and widespread active centres in catalysts and drugs. An analysis of their hyperfine and g-values provides detailed insight into their electronic structure and allows conclusions to be drawn about the reactivity of copper sites.



Of particular relevance are square-planar Cu(II) EPR centres in d_{x2-y2} ground state, which typically show paradigmatic EPR spectra with $g_{\parallel} > g_{\perp} \approx g_e$ and $|^{Cu}A_{\parallel}| \gg |^{Cu}A_{\perp}|$. In contrast, square-planar Cu(II) complex $[L^{pyNHC}Cu](PF_6)_2$ (L^{pyNHC} = macrocyclic bis(NHC)-bis(pyridine) ligand, **1**) exhibits a drastically different EPR spectrum with $|^{Cu}A_{\parallel}| \ll |^{Cu}A_{\perp}|$ (see **Figure 1**), whilst retaining the usual g-tensor pattern.

Figure 1 *(a) X-band, (b) Q-band, and (c) W-band EPR spectra of complex **1** in frozen solution and (d) liquid solution X-band EPR spectrum.*

Using a combination of multi-frequency EPR and W-band TRIPLE-ENDOR spectroscopy, we determine the exact g- and hyperfine values of **1**. In particular, we are able to determine the positive sign of the Cu HFS – opposite to the usually observed negative sign. The sign change explains the unusual hyperfine structure pattern in the EPR spectra and serves as a sensitive indicator of the electronic structure. An analysis based on quantum chemical calculations reveal that the sign reversal is due to strong 4s mixing in the ground state, caused by the donor strength of the ligand framework.

Talk:
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The effect of symmetry, vibrational excitation, spin-orbit coupling and hyperfine interaction on electron spin dynamics probed by magnetic deflection experiments

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Isolated tetrel clusters in the gas-phase containing a single paramagnetic dopant are suitable for systematically investigating the influence of symmetry, vibrational excitation, spin-orbit coupling and hyperfine interaction on electron spin dynamics. Stern-Gerlach as well as refocusing experiments are used for this purpose. The discussion of the observed spin dynamics is carried out with a model that takes avoided state crossings in dependence of the various parameters into account.

Talk:
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Ultralow-field NMR for biological and industrial applications: A tale of two cities

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In NMR literature, the term “ultralow field” (ULF) is commonly used to refer to magnetic fields below Earth’s field—the so-called hypogeomagnetic regime—such that magnetic shielding or active field cancellation is required in experiments. Another useful definition relates the magnetic field to the spin system under study: at ultralow field, the *J*-coupling between spins dominates interactions with the external field [1]. Beyond fundamental understanding of spin dynamics, these understudied regimes are relevant for diverse real-world applications—including spin biochemistry, chemical monitoring inside metal structures, field cycling, biomedical diagnostics, and even space exploration.

This talk will highlight several aspects: (1) methodology of ULF NMR using quantum detectors [2], (2) insights into spin relaxation at ULF [3], (3) recent studies on biological and industrial systems in Mainz and Berlin [4,5], and (4) the possibilities of ULF NMR for commercial EV-battery diagnostics.

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Talk:
58

Competing Defect Channels in Sequentially Implanted hBN: Nitrogen as a Bright-Vacancy Source and Oxygen as a Parasitic Sink

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Negatively charged boron vacancies in hexagonal boron nitride (hBN) are promising optically addressable spin defects for quantum sensing. Yet only on the order of 0.1% of irradiation-created boron vacancies have been estimated to occupy the optically active V_B^- charge state [1]. Improving their generation and charge-state control is therefore essential. We investigate how sequential nitrogen and oxygen implantation controls their optical and magnetic-resonance response, testing whether oxygen-related donors stabilize the bright vacancy charge state. A 1.5 micrometer-thick hBN flake was patterned with a 4 x 4 matrix of 12 kV nitrogen and oxygen doses from 6.24 x 10^{11} to 6.24 x 10^{14} ions cm^{-2}. We combined photoluminescence spectroscopy, zero-field optically detected magnetic resonance (ODMR), dark-time relaxation measurements, and temperature sweeps from 8 to 300 K.

Nitrogen implantation strongly increases the 700-850 nm emission and the integrated ODMR area, whereas oxygen suppresses both observables at high nitrogen dose and transfers spectral weight into the 600-700 nm band. Implantation also shortens the dark-time relaxation and introduces systematic changes in the zero-field splitting parameters D and 2E. A sequential latent-population model reproduces the photoluminescence and ODMR trends with R^2 above 0.93. Within this model, nitrogen creates the bright vacancy-related population about 3.4 times more efficiently than oxygen, while oxygen activates a strong parasitic conversion pathway that consumes this population.

At 8 K, 2E correlates closely with the ODMR-active population. On warming, 2E decreases by approximately 20 MHz and the correlation broadens, consistent with thermally activated redistribution of local charge. In contrast, D decreases smoothly with temperature and is described by spin-phonon renormalization with effective phonon energies of 16-19 meV, while implantation-dependent offsets remain.

The data therefore do not support an oxygen-induced enhancement of the bright boron-vacancy population under continuous green-laser excitation. Instead, nitrogen and oxygen provide distinct creation and redistribution channels. Species-selective implantation thus offers a route to engineer both the optical response and spin Hamiltonian of hBN defects.

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Talk:
59

Zero- to ultralow-field J-spectroscopy with a diamond magnetometer and applications in neurosurgery

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Dr. Arne Wickenbrock, Johannes Gutenberg-Universität and Helmholtz Institut Mainz, Mainz, Germany

Nuclear magnetic resonance (NMR) is a powerful tool for probing molecular structure and dynamics, but conventional high-field systems are bulky and suffer from field inhomogeneities. Zero- to ultra-low-field (ZULF) NMR overcomes these limits by exploiting internal spin interactions in a magnet-free, shielded environment. When combined with nitrogen-vacancy (NV) centers in diamond, it enables a compact, portable platform with high spatial resolution and broad bandwidth for noninvasive chemical sensing in microscopic volumes and real-world settings. We report detection of zero- to ultralow-field nuclear magnetic resonance (ZULF NMR) signals at frequencies of a few hertz using a diamond magnetometer. The sensing diamond is a truncated pyramid with 180 µm height and a 500^2 μm^2 base. The minimum stand-off distance is <1 mm, and the sensor sensitivity is 13 $pT/Hz^{1/2}$ at frequencies f above 5 Hz with 1/f-like behavior at lower frequencies. NMR signals were generated via signal amplification by reversible exchange (SABRE) parahydrogen-based hyperpolarization resulting in zero-field signals at 1.7 Hz and 3.4 Hz corresponding to the expected hetero-nuclear J-coupling pattern of acetonitrile. This work demonstrates a magnet-free platform for detecting chemically specific NMR signals paving the way for portable noninvasive diagnostics in microscopic sample volumes for biomedicine, industrial sensing through metal enclosures.
I will report the main results from [1] and sketch ways to deploy NV-based quantum sensors in real-world applications e.g. to help discriminating cancerous tissue during brain surgery.

Literature:

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Poster Abstracts

Poster:

1

Dissecting the influence of (multi)phosphorylation and GlcNAcylation on the regulation of phosphatases by proline isomerization within the CTD of RNA polymerase II

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RNA polymerase II (RNAPII) is a central enzyme in eukaryotic cells responsible for the transcription of protein-coding genes into messenger RNA (mRNA). The intrinsically disordered carboxy-terminal domain (CTD) of the largest subunit of RNAPII consists of multiple tandem repeats of the consensus heptapeptide $Y_1S_2P_3T_4S_5P_6S_7$, which forms a tail-like extension from its catalytic core. [1] The CTD is dynamically modified by many posttranslational modifications (PTMs) which play a key role in its activity and regulation. The association of PTMs including phosphorylation and glycosylation, with events in the transcription cycle gave rise to the concept of a CTD code. Recent studies show that the CTD code depends not only on PTMs but also on how regulatory proteins recognize specific CTD conformations. The phosphorylation status in the amino acids of the CTD is known to be depended on the isomeric state of adjacent prolines. [2] Proline *cis–trans* isomerism is a relatively slow conformational equilibrium due to the partial double-bond character of the amide bond restricting bond rotation.

Nuclear Magnetic Resonance (NMR) spectroscopy is well suited to study this phenomenon due to its ability to identify proline *cis–trans* isomers as distinct NMR signatures. We utilise chemically synthesised phosphorylated and glycosylated peptides of the YSPTSPS pattern with shorter chain lengths to investigate the influence of proline isomerism on posttranslational modifications in the CTD. By performing various 1D and 2D NMR experiments including $^{1}H–^{1}H$ NOESY, $^{1}H–^{1}H$ TOCSY and $^{1}H–^{13}C$ HSQC we could make resonance assignments and estimate the ratio of proline isomers within a given peptide of different modifications. Additionally, we aim to characterize the interactions between peptidyl-prolyl isomerase Pin1, and CTD short peptides by Saturation Transfer Difference (STD) NMR experiments. With these experiments we hope to arrive at insights that would help in cracking the so called CTD code.

Literature:

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Poster:

2

qNMR – Eine analytische Alternative zur HPLC in der pharmazeutischen Analytik

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Der Begriff quantitative NMR (qNMR) ist eigentlich ein Pleonasmus: Jede NMR-Spektroskopie ist aufgrund ihres physikalischen Messprinzips quantitativ. Die eigentliche Frage lautet daher nicht, ob NMR quantifizieren kann, sondern warum sie trotz dieser Eigenschaft erst heute als Alternative zur HPLC breite Anerkennung findet.

In den vergangenen zehn Jahren hat sich durch die enge Zusammenarbeit von Industrie, Hochschulen und Arzneibüchern in Europa, Nordamerika und Japan ein internationales Netzwerk etabliert, das die qNMR als leistungsfähige Alternative und Ergänzung zu chromatographischen Verfahren, insbesondere der HPLC, vorangetrieben hat. Zahlreiche Anwendungen wurden inzwischen in regulatorische und pharmakopöische Fragestellungen integriert.

Der Vortrag gibt zunächst einen Überblick über die Entwicklung dieser internationalen Initiative und deren Bedeutung für die moderne pharmazeutische Analytik. Anhand ausgewählter Beispiele aus der Wirkstoffcharakterisierung, Reinheitsbestimmung und Referenzmaterialanalytik werden die besonderen Stärken der qNMR hinsichtlich Rückführbarkeit, Universalität und metrologischer Qualität vorgestellt. Ziel ist es, das Potenzial der qNMR als eigenständige analytische Methode und als komplementäre Alternative zur HPLC aufzuzeigen.

Poster:

3

Quantum-Mechanical qNMR of Proteinogenic Amino Acids

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For the analysis of amino acids in food products or therapeutic proteins, HPLC is the predominant method. As an alternative, in this work, a foundation for the fast and semi-automated quantitative analysis of 15 proteinogenic amino acids following acid hydrolysis was established using quantum mechanical quantitative NMR (QM-qNMR).

Hydrolysis conditions were optimized, and solvent-related side reactions were identified and eliminated. pH-dependent ^{1}H iterative Full Spin Analysis (HiFSA) profiles were established for all relevant analytes, including a degradation product formed during hydrolysis. Quantification of the defined amino acid mixtures was achieved without derivatization or external calibration curves, that is needed for most chromatographic methods. Biases of up to 6% and relative standard deviations of up to 3% were achieved.

Four insulin analogues served as model proteins, exploiting their known stoichiometric amino acid ratios to determine recoveries without the need for an analytical balance. The four analogues were successfully distinguished based on their amino acid composition, and reproducible intraday recovery factors were determined for most amino acids. These results demonstrate the potential of QM-qNMR as a fast and calibration-free approach for amino acid analysis and establish an important basis for the future quantitative characterization of protein hydrolysates.

Poster:

4

In-situ NMR for the investigation of light-controlled anion-binding adaptive supramolecular systems

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Adaptive materials can not only induce changes in the properties upon exposure to external stimuli but also process feedback to regulate this response. Targeting the development of anion-binding supramolecular systems that exhibit adaptive behaviour in response to stimuli such as light, temperature, and salt addition, a series of tetra-triazole-based host structures containing a molecular switching unit have been synthesized. UV/Vis irradiation of these combined molecules with specific wavelengths enables *Z*-selective anion binding with a higher anion-binding constant than the *E*-isomer, thereby inducing photoreversible anion availability. [1]

The current project aims to investigate the influence of different functional units of novel hosts based on a diazocine switching unit and to optimize these systems concerning their anion-binding properties and isomer-selective binding behaviour. For this purpose, an *in-situ* NMR irradiation setup (Figure 1) is used. This setup enables irradiation and NMR measurements to be performed simultaneously, with LEDs connected to the NMR spectrometer via a glass fiber. *In-situ* irradiation NMR supports the investigation of the key characteristics such as switching efficiency, reversibility, and the photostationary state of each isomer form under different pulse sequences. In addition, anion-binding affinities are determined using NMR titration experiments under light irradiation, evaluated by the software Bindfit. [2]

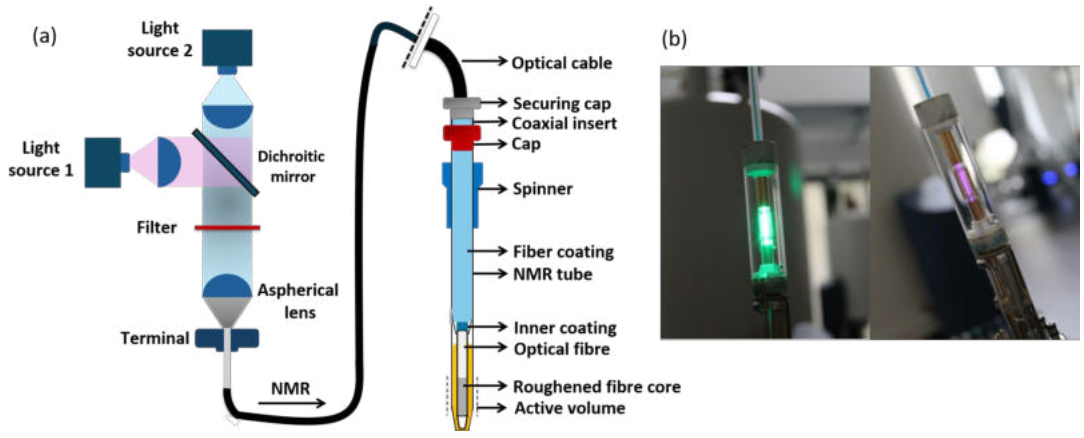

Figure 1. (a) Set-up for *in-situ* irradiation during NMR experiments. (b) Active sample volume during *in-situ* NMR irradiation (left: 520 nm green, right: 405 nm violet LEDs).

Literature:

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Poster:

5

Mapping of Dynamic Allostery within p38 Alpha Kinase via Network Analyses and NMR Spectroscopy*

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Kinases are major drug targets especially in cancer therapy. However, the high degree of conservation of their active sites hinders the development of selective inhibitors, motivating a deeper understanding of kinase conformational ensembles and allosteric communication pathways. Here, we use dynamical network analysis to identify key residues involved in a dynamic allostery between the N- and C-lobes that connects the major functional units of the MAP kinase p38α. By combining NMR spectroscopy, activity assays, and *in silico* analysis of wildtype protein and mutants in the presence or absence of an active-site inhibitor, we experimentally validate the obtained architecture with respect to global protein motion and long-range allosteric modulation. Notably, the identified network highlights communication pathways across several functional sites, prominently involving the allosteric site, the activation loop, and even the lipid-binding domain with its embedded cryptic pocket in the C-lobe. These findings provide mechanistic insight into p38α allostery and suggest viable opportunities for the rational design of allosteric modulators of MAP kinases.

**Nature Communications, just accepted.*

Selective WET Water Suppression Enables Quantitative Benchtop NMR Analysis in Protonated Solvents

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Benchtop NMR spectroscopy has emerged as a powerful analytical tool for routine chemical analysis due to its accessibility, low operating costs, and ease of use. A key advantage of benchtop NMR is the ability to analyse samples directly in protonated solvents, eliminating the need for expensive deuterated solvents and sample preparation. This enables rapid, on-the-fly measurements that can be readily integrated into routine synthetic chemistry workflows. However, the intense solvent resonance(s) often obscure nearby analyte signals, limiting accessible spectral information and making reliable spectral interpretation and quantification challenging. Here, we present a highly selective WET (Water suppression Enhanced through T_1 effects) solvent suppression approach optimised for routine benchtop NMR analysis [1]. The sequence efficiently suppresses the water resonance while preserving neighbouring analyte signals through a highly localised suppression profile. Signal perturbation is confined to a narrow sacrificed spectral window around the water resonance, while signals located more than 10 Hz away retain accurate intensities and integrals. This homogeneous excitation profile enables quantitative analysis despite the use of solvent suppression.

The quantitative performance of the method was first validated using a glucose/fructose mixture with an expected 50:50 molar ratio. All relative integrals were found to be in excellent agreement with the theoretical composition, demonstrating that selective WET suppression does not introduce integration bias outside the suppressed region. The observed α/β anomer ratio, determined from the relative integrals of the anomeric proton signals, was in good agreement with literature values, confirming the expected mutarotation of glucose [2,3]. The method was further applied to commercially available Coca-Cola® samples analysed directly without sample preparation. The resulting spectra enabled reliable sugar profiling and quantification from a single experiment, yielding a total sugar content of 12 g per 100 mL. The method was successfully implemented on a 100 MHz benchtop NMR spectrometer, demonstrating that highly selective and quantitative water suppression can significantly extend the capabilities of routine benchtop NMR for rapid analysis of complex samples in protonated solvents.

Literature:

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Poster:

7

An Investigation into the Standard Addition Method for the Quantification of Commercially Available Essential Oils via qNMR

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Quantitative NMR (qNMR) methods have emerged for the quantification of complex mixtures, namely essential oils. [1,2] In general, qNMR involves the use of an internal standard, external standard, chemometrics, and/or pairing with chromatography methods/mass spectrometry. [3,4] The use of the standard addition method for qNMR, while less common, may also be possible for the analysis of complex mixtures.

To investigate this method, linear and cyclic terpenes were characterized in commercially available essential oils and added in known concentrations to samples of the same oils. From the ^{1}H spectra, the relationship between the analyte concentration and the peak area may be used to elucidate the composition of the oil sample with respect to that analyte. Resolving crowded areas of the spectra for further quantification presents a challenge for further work on this topic.

Literature:

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From π-π-stacking to magnetic self-alignment: NMR investigation of concentration-dependent aggregation in a sterically frustrated hexabenzocoronene

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Chemical shift anisotropy is a well-known NMR phenomenon, e.g., for aromatic protons, whose anisotropic shielding arises from a field-induced ring current in the conjugated π-system.[1] This ring current also produces an anisotropy of the magnetic susceptibility (Δχ), which drives self-alignment that scales with $\Delta\chi \cdot B_0^2$ and is measurable once the π-system is large enough.[2]

Large π-systems also self-associate via a predominantly dispersive interaction commonly termed “π-π-stacking”,[3] which depends strongly on the aromatic structural motif and is well established in carbon-rich, solid-state, and supramolecular chemistry.

In this study, we observed concentration-dependent chemical shift changes for a sterically frustrated hexabenzocoronene (HBC),[4] fitting the data to monomer-dimer[5] and isodesmic[6] aggregation models. Both gave consistent association free energies ($\Delta G° = -14.04$ and -13.95 kJ/mol; $K = 289 \pm 27$ and 278 ± 17 M^{-1}, respectively) at the lower end of the typical range for aromatic π-π-stacking and well below the value expected for an idealized, unhindered HBC dimer,[7] consistent with steric frustration limiting π-overlap. The smaller fitting errors for the isodesmic model suggest a minor population of higher-order aggregates, though monomer and dimer remain the dominant species.

This raised the question of whether these aggregates measurably influence the self-alignment of such molecular motifs.

This was probed via CLIP-HSQC experiments[8] at 4 concentrations and 3 fields (400, 600, 900 MHz), measuring the total one-bond CH coupling ($^1T_{CH}$) of the aromatic protons. A field-dependent dipolar contribution of up to −3 Hz appeared at all concentrations; plotting $^1T_{CH}$ against B_0^2 for three of the six aromatic protons gave satisfactory linear fits, from which $^1J_{CH}$ (intercept) and a field-independent alignment slope were extracted. Error-weighted mean slopes were -5.27 ± 0.02, -4.79 ± 0.04, -4.56 ± 0.08, and -3.16 ± 0.53 mHz/T² for 18.8, 9.8, 6.0, and 1.6 mM, respectively, showing a monotonic increase of the dipolar contribution with increasing concentration.

Literature:

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Water Determination by NMR for Routine Control

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The water content of a product (for example, in the food or pharmaceutical industry) plays an important role in its stability [1] and is thus regularly controlled. For this, Karl-Fischer titration is predominantly used, for its high sensitivity and selectivity to water [2]. However, this method requires hundreds of milliliters of titration agent and sample, dissolved in specific solvents. On the other hand, NMR is used to confirm the structure and determine the purity of sample, with less than 1 mL of solvent and around 100 mg of product.
Moreover, water determination and purity evaluation are often run in parallel. While Karl-Fischer titration can only be used for water determination, NMR could be used to quantify both the sample and the water it contains. This raises the question: if NMR is already used to quantify the main compound, why can't it also be used to quantify water?
In this work, water determination with NMR was investigated on different samples, where the water signal is overlapped or not, and with different water content (ethanol, sugars and polypeptides). Results show that a difference between NMR and Karl Fischer of 1% or less in the water content can be obtained. Compared to a purity assessment, water determination only requires the acquisition of a blank (as solvents usually contain some amount of water), which takes only a few minutes.
Another interesting result from this work is that no additional chemical reference is needed to quantify the water. Instead, the ^{2}H signal of the solvent is used as the reference, which avoids any overlap with a chemical reference.

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Poster:

10

Multinuclear study of the correlation between pH and chemical shift in NMR

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NMR spectroscopy enables a comprehensive view into the chemical system of a sample under analysis, including a wide range of physicochemical information, and offers a powerful measurement method for the precise determination of pH and pD values in various chemical applications.

By using different nuclei (e.g., ^{1}H, ^{13}C, ^{31}P, as well as ^{15}N and ^{17}O) a multinuclear perspective on the sensitivity of chemical shifts to the protonation states of specific functional groups is achieved. Over a wide pH range, it demonstrates that the shifts in the measurable resonance frequencies of various nuclei correlate with the effective proton concentration of the sample solution.

The potential applications of pH measurement using NMR are diverse in chemical analysis and, in some cases, offer significant advantages even over conventional pH measurement methods due to the inclusion of multiple nuclei. The practical applicability of this NMR approach may be limited by factors such as lower sensitivity, greater complexity, and the overall cost of the measurement technology; nevertheless, this methodology contributes to the fundamental understanding of quantitative NMR spectroscopy and supports further research into a multinuclear approach for routine qNMR analyses.

Poster:
11

SPEAR Me, c-MYC: Toward the Structural Basis of Epigenetic Inheritance

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Gene activation is a critical process underlying cellular responses to developmental signals, environmental stimuli, and transitions between distinct cellular states. It is initiated by sequence-specific transcription factors that recruit chromatin-modifying enzymes and chromatin remodelers, thereby promoting chromatin accessibility at target genomic loci. Once activated, many genes remain transcriptionally active through multiple cell divisions, which is essential during processes such as cell differentiation, organogenesis, and tumorigenesis. A central question in epigenetics is how transcriptional states are maintained across mitotic divisions, enabling the inheritance of gene expression patterns in the absence of changes in the DNA sequence—commonly referred to as epigenetic memory.

In a recent study [1], we identified SPEARs (S-phase Early RNAs)—a novel class of long non-coding RNAs expressed during DNA replication that contribute to the maintenance of active chromatin states by facilitating the transfer of histone acetylation patterns. A key example is the proto-oncogene c-MYC. We observed that acetylation of its nucleosome-associated histones appears to be mediated by a SPEAR harbouring an evolutionarily conserved core motif—designated RM9. This 24-nucleotide sequence is expressed near nucleosomes and is proposed to simultaneously bind the histone monomer H2A.Z, the TIP60 complex (KAT5) and possibly also DNA. Upon binding, KAT5 acetylates H2A.Z at three distinct lysine residues on its N-terminal tail, thereby preserving the original acetylation pattern and equilibrium of acetylated H2A.Z throughout S-phase.

The molecular mechanisms underlying the interaction between RM9, KAT5, and H2A.Z are currently unknown and represent a critical gap in our knowledge. The structural basis of these interactions—particularly the conformational dynamics of RM9, its binding interfaces with KAT5 and H2A.Z, and the allosteric regulation of KAT5 activity—remains uncharacterized.

In this project, we aim to uncover the key molecular interactions of RM9 with KAT5 and H2A.Z. Our approach will begin with the detailed characterization of RM9 by high-resolution structural determination—using solution-state NMR spectroscopy—to resolve its three-dimensional architecture. These data will serve as a foundation for dissecting the molecular interface between RM9, KAT5, and H2A.Z, ultimately revealing how a short, conserved RNA motif can guide the precise re-establishment of histone acetylation patterns during DNA replication.

Literature:

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Poster:

12

Making the INADEQUATE Available: Ernst-Angle Excitation and Robust $^{13}C,^{13}C$ Double-Quantum Correlation

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The structure determination of organic molecules relies heavily on the unambiguous identification of carbon connectivities. The INADEQUATE experiment provides a powerful tool for tracing carbon backbones by directly correlating $^{13}C,^{13}C$ connectivities, making it particularly valuable for proton-sparse molecules. However, its application at natural abundance is severely limited by its intrinsically low sensitivity. Furthermore, the experiment is highly sensitive to variations in the $^{1}J_{CC}$ coupling, which can range from approximately 5 to 200 Hz, while the large spectral offsets encountered at high magnetic fields pose additional challenges for uniform pulsing.

Here, we present optimal-control-derived 45°, 60°, and 120° pulses designed for sensitivity-optimized INADEQUATE experiments in liquid state NMR. Building on these pulses, we introduce a set of INADEQUATE experiments that are simultaneously robust to variations in coupling, offset, and B_1 field strength, termed COB-INADEQUATE. Finally, we demonstrate both 1D and 2D $^{13}C,^{13}C$ eCOSY experiments at natural abundance, enabling sensitivity-optimized excitation using the Ernst angle.

Structural characterization of fractionated beech lignin using NMR spectroscopy and ultrahigh resolution mass spectrometry

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Lignin represents a vast, underutilized renewable source of aromatic compounds, yet its structural complexity and heterogeneity remain major barriers to targeted valorization. [1-3] Industrial pulping processes - particularly Kraft pulping - yield lignin combined with sugars, lipids, tannins, and other extractives, resulting in highly variable and impure materials that complicate purification and downstream chemical conversion.

To address this challenge, we investigated the molecular architecture of beech lignin obtained via Kraft pulping, employing a multi-fractionation strategy to probe compositional heterogeneity. Lignin was separated using solvent fractionation (water/acetone gradients), membrane filtration (varying pore sizes), and semi-preparative gel permeation chromatography (GPC), enabling isolation of fractions across molecular weight and polarity ranges.
Comprehensive structural characterization was achieved through combing NMR (HSQC, quantitative ^{13}C NMR) and ultrahigh-resolution tandem mass spectrometry. An overview of compound classes can be generated with 1D MS analyses of soluble compounds via electrospray ionization (ESI) and of the entire sample through graphite assisted laser desorption and ionization (GALDI). HSQC-NMR and neutral loss analysis from tandem MS shows that the investigated beech lignin consists predominantly of guaiacyl and syringyl units, which are mainly linked via β-O-4', β-β' and β-5' bonds. Accompanying substances such as sugars, lipids, and tannins were detected in NMR and MS analyses, emphasizing the complexity of the samples. Tandem mass spectrometry was further used to investigate structural differences of characteristic precursor ions in different extraction mixtures by correlating the neutral losses after collision induced dissociation.

The combination of NMR spectroscopy and mass spectrometry proved to be complementary and provided consistent results on the structural composition of the beech lignin analyzed. These initial analyses of the molecular organization and linkage patterns represent the first step toward fully realizing lignin's potential as a renewable resource, paving the way for its higher-value applications beyond mere energy production.

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Poster:

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Development of a NMR and MS-based tool for automated metabolite identification in complex mixtures

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The unambiguous identification of chemical components from complex mixtures is essential for mechanistic and variety interpretation in metabolomics-based classification tasks, such as food authentication or biomedical differentiation. While Proton Nuclear Magnetic Resonance (NMR) spectroscopy offers a non-destructive measurement and extensive structural information, metabolomics samples often contain a multitude of components, causing highly overlapping signals. This makes NMR peak assignment difficult, especially for unknown compounds.

This project therefore expands on SCORE-metabolite-ID, a correlation-driven tool for identifying known and unknown substances in complex mixtures. Its central idea is to correlate signals originating from the same metabolites along the chromatographic time axis using ^{1}H-NMR and direct injection mass spectrometry (DI-MS). The spectra are aquired offline and in parallel based on LC fractionation, causing signals to experimentally deconvolute. [1] By leveraging the so called extracted delta and extracted mass chromatograms (EDC/EMC), the workflow aims to assign peaks and identify metabolites independently of prior assumptions and data base matching, supporting identification of unknown compounds. To improve tool robustness when faced with real NMR metabolomics data, the project focuses on key technical aspects like improved spectral alignment and computational deconvolution to untangle overlapping NMR signals so that signal-to-metabolite assignments become more reliable.

Furthermore, the above workflow will be coupled with ^{1}H-NMR based chemometric analyses to allow for metabolomics classification tasks and Surrogate Minimal Depth (SMD) based variable selection and relation analysis. [2] The combination of these two approaches will lead to a generally applicable and automated tool, improving the understanding of metabolomics datasets by providing an accurate identification of class-specific metabolites, potentially leading to the discovery of yet unknown metabolites and pathways.

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Poster:
15

NMR-Based Studies on the Structure-Activity Relationship of Antimicrobial Peptides

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The rapid global rise of antibiotic resistance necessitates the development of new therapeutic strategies, with antimicrobial peptides (AMPs) representing a promising class of drug candidates. Building on our previous identification of two active AMPs, we performed an extended structure–activity relationship (SAR) analysis to dissect the relative contributions of hydrophobicity, secondary structure, and conformational constraint to antimicrobial efficacy [1]. Systematic amino acid substitutions were introduced into linear peptides to modulate hydrophobic surface area, while peptide cyclization was achieved *via* triazolyl bridges with varied position and ring strain. Antimicrobial activity assays revealed that increasing the hydrophobic surface in linear peptides consistently enhances antimicrobial potency. Likewise, in triazolyl-bridged peptides, increased ring strain generally correlates with improved activity, although both the position and orientation of the triazole bridge exert a pronounced influence on efficacy. NMR spectroscopy showed that linear peptides adopt predominantly random-coil conformations in aqueous solution, whereas N-terminal triazolyl cyclization induces partial α-helical structure. To rationalize these findings at the molecular level, we compared triazolyl-bridged peptides with their linear analogues using solution and micelle-bound NMR. Triazole-mediated prestructuring stabilizes a well-defined α-helix and promotes amphipathic surface organization, characterized by spatial segregation of hydrophobic residues and a contiguous positively charged surface. Collectively, our results demonstrate that while α-helical preorganization and amphipaticity enhance antimicrobial activity, the dominant driving force remains the extent and distribution of hydrophobic surface area. Fine-tuning hydrophobicity and conformational constraint through targeted substitutions and triazolyl cyclization emerges as an effective strategy for optimizing AMP activity.

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Quantification of crRNA bound to Cas13a by Pulsed Electron-Electron Double Resonance

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Cas13a is a class 2 type VI CRISPR-associated RNase involved in the immune response of prokaryotes against foreign genetic elements. Exploring the structure-function relationship of Cas13a is necessary to understand the mechanism of RNA binding to the protein and its nuclease activity. While experimental structures of Cas13a along its mechanistic pathway are reported, [1-3] they stem from different species, meaning there is no complete understanding of the mechanistic pathway of Cas13a from a single bacterium. Additionally, these structures do not give information on conformational dynamics in a certain state along the mechanistic pathway and neither can binding parameters such as dissociation constants or rate of RNA binding to the protein be derived. Standard techniques to obtain binding parameters in biological systems include isothermal titration calorimetry (ITC), biolayer interferometry and fluorescence polarization anisotropy. [4-6]

In this study, we use pulsed electron-electron double resonance (PELDOR, also called DEER) [7] to resolve conformational dynamics in apo and CRISPR-RNA (crRNA) bound state and also observe the binding of crRNA to Cas13a from *leptotrichia buccalis* in dependence of both the crRNA excess and time. The time resolution is achieved by employing microsecond freeze hyperquenching (MHQ). [8]

This approach yielded a dissociation constant of the crRNA-Cas13a complex that is in agreement with results from ITC measurements. Furthermore, the results indicate that the binding of crRNA to Cas13a at a low crRNA excess happens on a time scale spanning 7 orders of magnitude, from roughly hundred microseconds to hundreds of seconds.

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Poster:

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Protein unfolding and aggregation at all stages as seen by NMR

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Protein misfolding and aggregation is closely linked to many neurodegenerative diseases like Alzheimer's or Parkinson's disease, and understanding the underlying processes like protein (un)folding, aggregation and fibril formation is a rewarding challenge. Here we demonstrate the enormous potential of NMR-Spectroscopy at all time-scales ranging from solution NMR, HR-MAS via room-temperature solid-state NMR to DNP enhanced low-temperature NMR in frozen solutions for the study of protein folding, unfolding and aggregation [1].

On the one hand, the structure and molecular details of amyloid fibrils can be studied by solid-state NMR-spectroscopy [2-6]. We also apply a multidisciplinary approach combining solution-NMR, in-situ MAS NMR-spectroscopy and DNP-enhanced NMR solid-state NMR-spectroscopy of frozen solutions to follow and characterize the process of unfolding, oligomerization and protein aggregation of the model protein PI3K SH3 in real time and with high resolution [7]. In particular, we exploit DNP-enhanced solid-state NMR-spectroscopy of frozen solutions to determine structural ensembles of backbone and side-chain conformations of well-folded, unfolded, intrinsically disordered and fibrillated proteins [8-11], which are linked to aggregation kinetics and products at different conditions.

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Poster:

18

Impact of Methionine 35 Oxidation on Monomer Conformational Dynamics and Fibril Formation of Amyloid-beta

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A characteristic feature of Alzheimer's Disease is the deposition of neuritic plaques in the central nervous system, which consist primarily of highly ordered amyloid fibrils formed by aggregation of largely disordered amyloid-beta (Aβ) monomers. Another important factor appears to be oxidative stress [1]. Methionine 35 (Met35red) in Aβ can be oxidized to methionine sulfoxide (Met35ox) [2] and Aβ Met35ox is detectable in neuritic plaques [3]. Met35 oxidation modulates the conformational ensemble of Aβ monomers and interferes with fibril formation [4]. To investigate these effects in more detail, we compared the structure, dynamics, and fibril formation of Aβ(1-42) M35ox vs. M35red in 28% acetonitrile at acidic pH. SSP [5] analysis of the ^{13}C chemical shifts reveals that the transient C-terminal β-hairpin propensity of Aβ(1-42) M35red monomers [6] is amplified by these buffer conditions, which are particularly conducive to fibril formation in vitro [7]. This partial order is reflected in increased ^{15}N NMR relaxation rates and $\{^1H\}^{15}N$ heteronuclear NOE values in the C-terminus of Aβ(1-42) M35red. By contrast, the C-terminus of Aβ(1-42) M35ox is highly disordered, suggesting that the increased hydrophobicity of methionine sulfoxide destabilizes the C-terminal β-hairpin. Aggregation was monitored by quantifying the decrease in soluble monomer signal intensity in a series of $[^1H,^{15}N]$ HSQC NMR spectra over time at a temperature of 5°C. The relatively rapid Aβ(1-42) M35red monomer decrease shows complex kinetics with several stages. By contrast, the kinetics of Aβ(1-42) M35ox monomer loss is consistent with a markedly slower mono-exponential process that leaves about 8% of residual detectable monomer signal even after many months. Similarly, Aβ(1-42) M35ox aggregation exhibits a significantly longer lag phase, slower exponential fibril growth, and lower equilibrium fluorescence compared to Aβ(1-42) M35red in thioflavin-T (ThT) assays at neutral pH and a temperature of 30°C. After monitoring the monomer loss at 5°C for several months, the aggregates that had formed in the NMR samples were analyzed by transmission electron microscopy (EM). The structure of Aβ(1-42) M35ox fibrils was determined by cryo-EM for comparison to the fibril of structure of Aβ(1-42) M35red published previously [7].

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Poster:

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Structure of the full-length YopO-SycO complex based on native mass spectrometry and EPR spectroscopy

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The *Yersinia* outer protein O (YopO) is one of six effector proteins of the pathogenic *Yersinia* bacteria, including the plague-causing *Yersinia pestis* bacteria. It is a key component in the suppression of the hosts' immune response upon infection. YopO is comprised of three domains, a GDI, a kinase, and a membrane localization domain. During the infection process, the specific Yop chaperone O (SycO) is hypothesized to bind as a dimer to the membrane anchor thereby masking it and aiding to the solubility of full-length YopO [1]. While structures of YopO without the membrane anchor have been solved [2,3], this is neither the case for full-length YopO nor for the full-length YopO-SycO complex. We therefore aim here to gain insights into the structure and formation of the full-length YopO-SycO complex.

We were able to express, purify and subsequently spin label isolated SycO and the full-length YopO-SycO complex. This enabled us to obtain structural information of the protein complex, using pulsed EPR spectroscopy, namely pulsed electron electron double resonance (PELDOR or DEER) [4]. Based on the obtained EPR data, structural models of the full-length YopO-SycO complex were created in combination with AlphaFold3.

The obtained PELDOR data indicates formation of higher SycO oligomers in the full-length YopO-SycO complex, whereas the literature hypothesizes a dimeric state (full-length YopO-$(SycO)_2$). We will present structural models of a possible full-length YopO-$(SycO)_3$ and YopO-$(SycO)_4$ complex, calculated based on the EPR data. Native mass spectrometry verified the formation of trimeric and tetrameric SycO in the full-length YopO-SycO complex.

Literature:
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syncDIPSHIFT – a new method for investigating molecular orientations

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Macromolecules in polymeric materials become partially oriented when the sample is subjected to mechanical loading, such as stretching or compression. The degree of orientation largely determines the macroscopic properties of the material. To experimentally confirm structure–property relationships, absolute values characterizing the degree of chain deformation are required. Anisotropic spin interactions enable NMR investigations in this field. Three conditions must be fulfilled to determine the orientation moments of the macromolecular segments: (i) the interaction tensor, including its orientation within the molecule, must be known; (ii) the interaction anisotropy must be on the order of the spinning speed required for sufficient spectral resolution; and (iii) the orientation of the specific atomic group within the segment must be known.

The syncMAS method [1] exploits chemical shift anisotropy (CSA). For the investigation of oriented polycarbonate (PC), however, it is not possible to fulfil all three conditions to a sufficient extent. The CSA of the methyl carbons is relatively small, while neither the spatial orientation of the aromatic rings nor the CSA of the carbonate carbon is known with sufficient accuracy. Although syncMAS investigations of PC reported in the literature provide orientation data, their accuracy is limited for the reasons outlined above.

A possible solution is an experiment that exploits dipolar interactions instead of CSA. The dipolar tensor is defined by the length and direction of the CH bond, thereby fulfilling condition (i). The CH dipolar interaction can be monitored site-selectively using the 2D DIPSHIFT pulse sequence [2]. The dipolar information is contained in the curves between the rotational echoes in the indirect dimension. We combined this approach with rotor synchronization to obtain a 3D experiment, in which the time dimension t_2 corresponds to the duration of the Lee–Goldburg (LG) decoupling, while t_3 is the acquisition time. The time dimension t_1 is proportional to the angle between the sample director and the plane spanned by $\mathbf{B_0}$ and the rotor axis at the beginning of the pulse sequence. The dependence on t_1 provides information about the sample orientation. This effect is most pronounced when the LG decoupling is centered halfway between the rotational echoes, for example at $t_2 = T_{rot}/2$. By fixing this condition, the experiment can be reduced to two dimensions. Condition (ii) is likewise fulfilled. We defined the segment vector as the normal to the $C(CH_3)_2$ plane and, based on this definition, determined the orientation moment of the segments. As an additional benefit, the method also provides information on molecular geometry, such as ring rotation angles.
This method appears to be particularly well suited for investigating aliphatic carbons.
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Poster:
21

Polymer Composition of Recycling Feed

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The increasing use of complex mixed waste streams in mechanical recycling requires robust analytical methods for quantitative polymer composition determination. In this work, automotive shredder residue (ASR) was used as a representative heterogeneous feedstock to develop and evaluate NMR-based quantification strategies. A workflow combining cryogenic milling for sample homogenization with both solution-state and solid-state NMR spectroscopy was established, enabling analysis of a broad range of polymers independent of molecular weight, branching, or crosslinking. For solid-state NMR, quantification of polymer contributions in mixed samples with spectral crowding was enabled by linear decomposition into reference spectra. The presented methodology provides an approach transferable to other mixed recycling feedstocks and is intended to generate reliable reference data for qualification of higher-throughput analytical methods rather than routine process control.

Poster:

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Multiscale Transport in Anion Exchange Membranes Probed via Pulsed Field Gradient NMR

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Anion Exchange Membranes (AEMs) have recently emerged as a promising ionomer, enabling green hydrogen production with noble-metal-free catalysts. However, limited insight into their microstructure calls for advanced characterization techniques. Pulsed Field Gradient Nuclear Magnetic Resonance (PFG-NMR) offers significant potential for elucidating the transport microstructure of membranes, providing valuable insights for their rational synthesis. To obtain information about the spatial organization of the membrane that would be averaged out in a conventional single-point PFG-NMR measurement, the evolution of the proton self-diffusion coefficient with increasing diffusion time was characterized in a diffusion dispersion experiment, which enabled the transport to be probed over progressively larger time and length scales. [1] To demonstrate the applicability of this experiment to AEMs, three benchmark membranes composed of distinct polymeric materials were investigated. The membranes were conditioned according to two well-defined protocols, achieving low and high water uptake.

Initial analysis of the diffusion dispersion curves revealed pronounced differences at short length scales, but convergence at length scales comparable to the membrane thickness, revealing that transport is governed not only by local polymer chemistry but also by the membrane's hierarchical structure. Insightful parameters related to membrane microstructure could be extracted by fitting the dispersion curves with a Hill-type equation. Analysis of the fit results highlights the critical influence of membrane history and macroscopic water uptake in modulating confinement effects. However, a dependence of the measured self-diffusion coefficient on the applied gradient parameters was observed, indicating that conventional Stejskal–Tanner analysis based on mono- or biexponential fitting is insufficient to capture the underlying distribution of diffusion coefficients. To resolve the distinct populations associated with heterogeneous environments within the AEMs, inverse Laplace transformation (ILT) of the PFG-NMR signal attenuation was employed. [2] The inversion uncovers two main modes with low and high mobility, attributed to water molecules near and far from the ionomer cationic groups, respectively. Together, these results demonstrate how transport heterogeneity and confinement are linked to AEM composition and hydration, providing a basis for rational membrane design, as will be discussed in the contribution.

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Poster:

23

Temperature- and Concentration-Dependent Ion Dynamics in $NaPF_6$-Based Liquid Electrolytes detected by NMR

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The rapidly growing demand for batteries calls for scalable energy-storage technologies beyond conventional lithium-ion systems. Sodium-ion batteries have emerged as a complementary technology to lithium-ion systems, combining abundant and widely available raw materials with the potential for lower costs, more resilient supply chains, and large-scale deployment [1,2]. While commercial Na-ion cells are already available, realizing the full potential of this technology requires a detailed understanding of the electrolyte, which governs ion transport, solvation and chemical stability. To address this knowledge gap, we present a systematic study of liquid electrolytes consisting of $NaPF_6$ in EC:PC. Salt concentrations between 0.2 and 1.5 mol/l are investigated over a temperature range from 283 to 343 K.

The main focus is on the temperature- and concentration-dependent self-diffusion coefficients of Na^+, PF_6^- as well as the solvent components EC and PC, determined by ^{23}Na, ^{19}F and ^{1}H PFG-NMR. In contrast to conductivity measurements, PFG-NMR enables the mobility of individual electrolyte species to be resolved separately. Water, HF and further degradation products are monitored to assess their potential influence on the diffusion measurements. Raman spectroscopy complements the NMR measurements by revealing changes in coordination and interactions between electrolyte species through the evolution, shifts and emergence of vibrational modes.

The temperature- and concentration-dependent self-diffusion of the individual electrolyte species provides insight into changes in ion association, cluster formation and solvation environments. Combined with spectroscopic information on electrolyte composition and degradation, these measurements help to elucidate the interplay between transport, interactions and chemical stability, providing a basis for the targeted optimization of liquid electrolytes for sodium-ion batteries.

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Poster:

24

Lab-Tools NMR techniques to measure porosity of rocks and viscosity of the recovered liquids.

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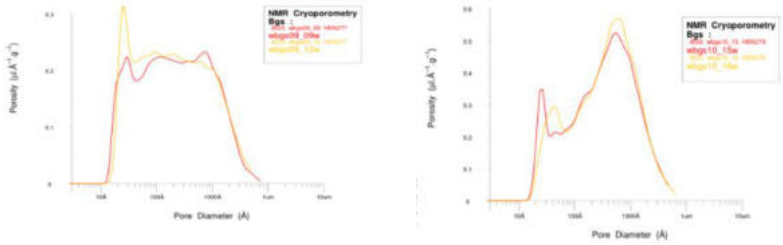
Gibbs–Thomson equation for the melting point depression, *Tm*, for a small isolated spherical crystal, of diameter *x*, in its own liquid, may be expressed as [1] :

$$\Delta T_m = T_m^{\infty} - T_m(x) = \frac{4\sigma_{sl}T_m^{\infty}}{x\Delta H_f \rho_s}$$

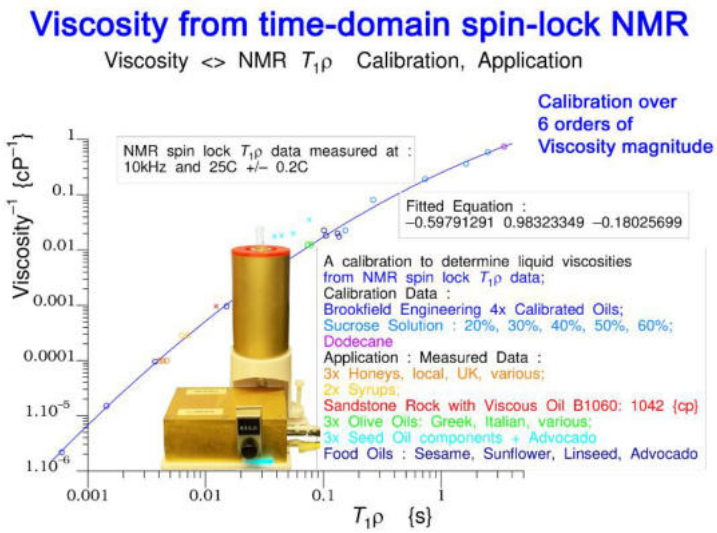
Using this Cryoporometric technique, we have measured pore-volume and pore size distribution on 10 samples of North Sea sandstone porous rock, from the National Geological Repository at the British Geological Survey (UKRI).



Cryoporometric Pore Size Distributions for 2 Sandstones.

We have also developed a novel technique for determining quantified viscosity, using NMR T1ρ [2], and measured the quantity and viscosity of the as-recovered liquids in the porous rocks.

Blue dots : Viscosity <> T1rhp Calibration Data, then applied to measure the viscosity of other samples in the bulk and in the rock pores, using our NMR spectrometers [3].



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Poster:

25

Dissolved or not? Low-field NMR relaxation insights into the microscale mobility of polymers in disperse systems

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Whether a polymeric component in a disperse system is (fully) dissolved or not may come with important implications on the process behaviour, the formulation stability or also on the regulatory assessment of the respective substance. While the differentiation of “liquid” (i.e. dissolved) or “solid” polymer seems to be quite straightforward on the macroscale, these classical approaches such as ASTM D4359 cannot be applied to polymers within a disperse formulation. Also other classical approaches to assess solubility such as OECD guideline 120 are hard to apply to disperse formulations due to issues such as high viscosity or turbidity of the formulation.

In a recently published paper [1], we suggested to use information from T2 measurements as a fast and simple tool to assess the microscale dissolution state of polymers in such formulations. To this end, we have introduced a simple index (restricted mobility index, RMI) based on the ratio of time averages values of different regions of the solid echo decay as a metric for microscale mobility restriction in polymer-containing formulations. No fitting and no inverse Laplace transform is needed for this index, avoiding both subjective decisions on the selection of fitting models and the numerical instabilities that come with ILT evaluations. Using the system polyvinyl pyrrolidone - water as an example, the change of the index and of the water phase relaxation properties over the transition from dissolved polymer to water-swollen solid polymer could be demonstrated.

The sensitivity of the index to the presence of non-dissolved proton populations in liquid samples was studied using a series of model samples produced from solid sugars and plant oils. Using these samples, a sensitivity of about 0.1% non-dissolved protons inside a liquid phase could be demonstrated. Furthermore, we applied the RMI also to the melting of thermoplast materials where we could demonstrate an excellent agreement with DSC data. Also, the partial dissolution of hard-to-dissolve polymer such as cellulose in benign solvents such as water/NaOH could be compared on the basis of the RMI.

Due to its simplicity, the RMI concept is also very well fitted for use in big data and high-throughput screening systems.

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Poster:

26

Synthesis and Characterization of a Binding-Activated, Light-Induced EPR Spin Label

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Pulsed Dipolar EPR spectroscopy is a method for measuring distances between spin labels. Traditionally, this is achieved by using two stable radicals or metal centers.[1] In contrast, light-induced spin labels can be switched from an EPR-silent state to an EPR-active state by a laser pulse, making the spin label detectable only when required.[2] Rose Bengal is an already established light-induced spin label, which has a high triplet yield, enabling large EPR signals.[3] The previously published Rose Bengal label, however, is attached via a long maleimide linker, causing undefined distance distributions.[3] Therefore, we aim to develop a short-linked Rose Bengal maleimide label.

We successfully synthesized a short-linked ethylene Rose Bengal maleimide (SLERB-M) featuring a linker design that is readily adaptable to a variety of other chromophores. To mimic covalent binding, L-Cysteine was linked to the maleimide (SLERB-M-Cys). The resulting compounds were characterized by optical spectroscopy and time-resolved EPR (tr-EPR) measurements.

Fluorescence spectroscopy measurements of all three components revealed quenching of the fluorescence of the maleimide-substituted Rose Bengal while attachment to the cysteine recovered the fluorescence. Tr-EPR measurements showed the same trend, with the triplet-state signal of SLERB-M being almost completely quenched, while Rose Bengal and SLERB-M-Cys displayed strong signals. Thus, the label is EPR-active only upon binding, and residual unbound label is nearly EPR-silent.

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Improved Sensitivity of EPR and DNP Methods with Home-made Probeheads

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Recently achieved enhancements in liquids by solid effect DNP at high magnetic fields [1, 2] have initiated strong interest in possible applications of the method to biomolecular research. Here we present a DNP probehead and new results for liquid-state DNP at 9.4 Tesla by combination of the Fabry-Perot resonator for microwave excitation at 263 GHz and a coplanar line for NMR detection that offers unique opportunity to study aqueous solutions of biological samples at physiological conditions [3]. Besides, we report sensitivity of a Q-band EPR spectrometer improved by factor of 2.5 with a new probehead by using the combination of a bimodal resonator with an additional low noise detection amplifier. The probe design is fully compatible with Bruker ELEXYS EPR spectrometers [4].

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EPR spectroscopy in the investigation of polyphosphazene-based organic radical batteries

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Organic radical batteries (ORBs) are a novel and actively developed class of thin, flexible, sustainable batteries capable of providing intermittent high currents as required for various applications, such as Internet of Things (IoT) devices. A new type of polymer investigated as possible ORB cathode with a polyphosphazene backbone (PPZ) bearing nitroxide radicals has been introduced recently [1]. It has a reported theoretical capacity of 131 Ah kg^{-1}, and it offers the possibility to tune its physicochemical characteristics by adding a wide variety of side groups to the polymer chain. Electron paramagnetic resonance spectroscopy (EPR) is the optimal method to investigate processes in radical polymers because its various methods allow the measurements of spin densities in samples, distinguishing between different interactions between spins and environment and study of redox processes involving radicals in operando. Recent studies [2] gave insight into the radical distribution within the organic radical cathode and the contact between active materials and conductive additive. In correlative investigations of new materials that include electrochemical studies and simulations, EPR can play an important role in developing an understanding of electron transfer mechanisms within an electrode, which opens a path towards improvement of battery performance [3].

Here, EPR is combined with electrochemical characterization and atomistic simulations to investigate newly synthesized PPZ- and cyclotriphosphazene-based polymers containing 2,2,6,6-Tetramethylpiperidinyloxyl (TEMPO) radicals. Their performance as cathode material has been tested, and theoretical capacity was compared with caculated spin density. Difference between theoretical and effective capacity and its tie to the level of crosslinking is discussed. Simulation of cathode composites with a distribution of radical and cationic forms of TEMPO has been performed. Existence of spin clusters with high radical density, impenetrable by solvents, is observed in both polymer materials, with estimated effective spin-spin relaxation time of less than 30 ns, which corresponds to strong interspin interactions. In such cases, experimental limitations prevent use of pulse EPR of radicals at high concentration or at room temperature. In order to overcome instrumental limitations of a spectrometer, longitudinal detection in EPR is discussed as method of electron transport in PPZ-based cathode materials. The data obtained as a result may contribute to the complex investigation of PPZ-based polymer cathodes with subsequent optimization of their composition and performance.

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Poster:

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Disentangling Spin-Label and Protein Conformations in PDS EPR

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Pulse dipolar electron paramagnetic resonance (PDS EPR) spectroscopy [1] combined with site-directed spin labelling (SDSL) is a powerful method for measuring distances in biomolecules in the nanometre range. PDS provides probability distributions of interspin distances and thus enables the investigation of the coarse-grained structure and structural changes of biomolecules such as proteins. However, the PDS-derived distance distribution reflects not only the biomolecular structure but also the conformational flexibility of the spin label, and disentangling these two contributions is non-trivial [1, 2].

The most widely used spin label is the methanethiosulfonate spin label (MTSSL) [3], which reacts with a cysteine residue of a protein and forms a three-bond-long linker between the protein backbone and the nitroxide moiety (Figure 1a). The recently proposed bromoacrylaldehyde spin label (BASL) [4, 5] forms a single-bond-long thioether linker upon conjugation to a cysteine residue (Figure 1b), which is expected to result in lower rotational flexibility compared with MTSSL. In addition to the shorter linker, the thioether bond formed by BASL is more stable than the disulfide bridge formed by MTSSL, which potentially broadens the scope of applications.

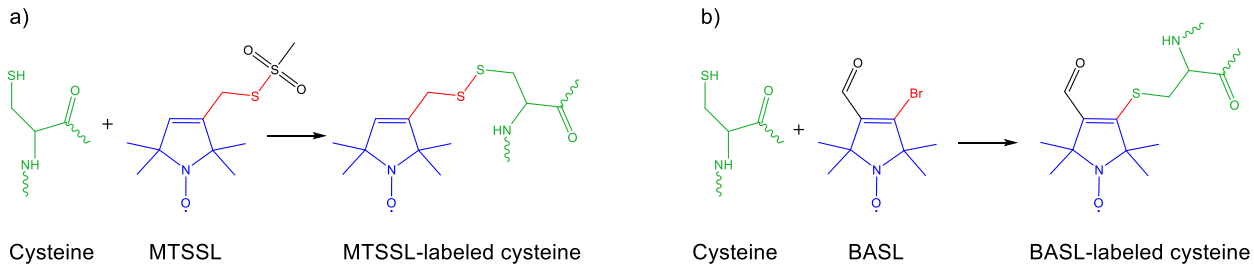

Figure 1: Cysteine-selective nitroxide spin labels. The cysteine residue is shown in green, the nitroxide group in blue, and the linker in red. a) The most commonly used nitroxide spin label MTSSL has a three-bond-long linker. b) The linker of the alternative nitroxide spin label BASL is only one bond long and therefore has lower rotational flexibility.

Herein, we investigate the influence of linker length on the width and shape of the PDS-derived distance distributions by comparing MTSSL and BASL using the *Yersinia* outer protein O (YopO) as an example.

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Poster:

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Characterization of 2,7,12,17-tetra-*tert*-butyl-Porphycene and it's Pd^{2+} complex: from synthesis to the photoexcited triplet state

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Porphycenes as constitutional isomers of porphyrins require a more demanding synthesis but exhibit fascinating and useful properties. In free-base porphycenes, tautomerism in the ground state and strong fluorescence from the photoexcited singlet state is established. [2] Production of Reactive Oxygen Species (ROS) via the photoexcited triplet state is observed for both free-base and metalloporphycenes. [3] These aspects have been extensively studied, whereas the properties of the photoexcited triplet states remain underexplored. Here we present an improved synthetic protocol and characterization of 2,7,12,17-tetra-*tert*-butyl porphycene and its Pd^{2+} complex. We characterize the ground states of both compounds with cyclic voltammetry and UV/VIS spectroscopy, and use transient EPR (trEPR) spectroscopy to investigate their photoexcited triplet states. For free-base porphycene, tautomerization effects are observed via temperature-dependent trEPR measurements, whereas these are absent in the Pd^{2+} complex. The zero-field splitting (ZFS) parameters demonstrate a retained π-π*-character for the Pd^{2+} complex. In contrast, a reorientation of the spin polarization from in-plane for the free-base towards out-of-plane for the Pd^{2+} complex is observed. The experimental data is complemented by DFT and CASSCF calculations. These results form a basis for selective modification of the porphycene macrocycle to control its triplet properties. These are relevant for applications such as photodynamic therapy (PDT) or spin polarization transfer via the radical triplet pair mechanism (RTPM).

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Electronic Substituent Effects on Pancake Bonding: Solution-Phase Dimerization Equilibria of Phenyl- and Fluorophenyl-Dithiadiazolyl Radicals

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Substituent effects on the dimerization of 1,2,3,5-dithiadiazolyl (DTDA) radicals have been studied extensively in the solid state, yet crystal packing forces obscure the intrinsic electronic contribution to pancake bond strength. Here we present the first pairwise solution-phase comparison of 4-phenyl-1,2,3,5-dithiadiazolyl (1) and 4-(perfluorophenyl)-1,2,3,5-dithiadiazolyl (2) using temperature-dependent UV-Vis spectroscopy, multi-frequency continuous-wave EPR spectroscopy and Mims-ENDOR spectroscopy. Van't Hoff analysis in toluene yields dimerization enthalpies of $\Delta H = -28.9$ kJ mol−1 for 1 and $\Delta H = -19.5$ kJ mol−1 for 2, showing that perfluorination of the aryl substituent weakens the π*–π* pancake bond by approximately 9 kJ mol−1. CW-EPR analysis reveals a small decrease of about 2% in the 14N hyperfine coupling upon perfluorination (room-temperature Aiso = 14.6 vs 14.4 MHz; 80 K Azz = 39.6 vs 38.7 MHz). Q-band Mims-ENDOR further resolves the individual ring-substituent couplings and shows that the 19F isotropic hyperfine constants of 2 (Aiso up to 5.7 MHz) exceed the 1H couplings of 1 (Aiso ≤ 2.0 MHz) by up to a factor of five, providing direct experimental evidence for a redistribution of SOMO spin density from the DTDA heterocyclic core onto the perfluorinated aryl ring. DFT calculations qualitatively reproduce the observed hyperfine trends and provide a positional assignment of the individual ring-substituent couplings. The influence of the solvent dielectric on the dimerization thermodynamics is additionally assessed by systematic variation of the solvent composition. Both radicals were obtained by a novel metal- and solvent-free route in which elemental sulfur itself reduces the dithiadiazolylium chloride during sublimation.

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Poster:

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

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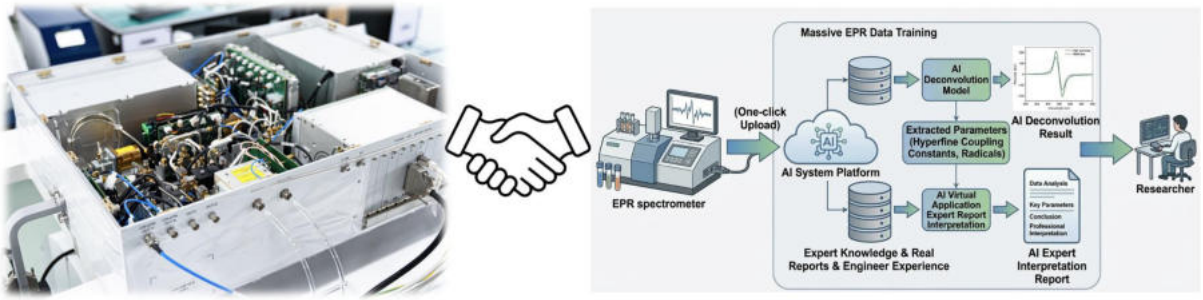

The advancement of Electron Paramagnetic Resonance spectroscopy is increasingly defined by the convergence of robust hardware and intelligent software. While EPR remains a vital tool for probing paramagnetic centers, broader adoption is limited by instrument complexity and the steep learning curve of 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.

Poster:

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Transport Properties of Solvate Ionic Liquids with Water as Co-Solvent

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Solvate ionic liquids (SILs), consisting of an oligoether ("glyme") and a weakly interacting Li salt, are promising electrolyte systems for the development of more sustainable batteries with improved transport properties. Due to their unique coordination structure of the lithium cation, they can exhibit superior transport behavior compared to conventional lithium salt electrolytes, which are often only partially soluble in organic carbonate solvents.

In this study, SILs consisting of various lithium salts and coordinating solvents were mixed with water as a co-solvent to investigate the influence of water content on transport properties and lithium coordination. Raman spectroscopy was used to determine the minimum fraction of free glyme after water addition. Pulsed-field gradient NMR (PFG-NMR) was applied to determine the diffusion coefficients of the electrolyte constituents. Additionally, electrophoretic NMR (eNMR) was used to measure the mobilities of ions and glymes, which coordinate lithium ions and therefore also migrate under an applied electric field. Furthermore, the ionic transference numbers were determined based on these mobilities.

The results show that increasing water content generally improves the transport properties of the investigated electrolytes, leading to higher diffusion coefficients and mobilities. In addition, both the anion and the coordinating solvent strongly influence the transport behavior and coordination structure. Smaller anions improve transport properties due to reduced viscosity, whereas longer glyme chains and cyclic ligands such as crown ethers decrease ion transport due to increased viscosity.

In conclusion, this study bridges the gap between conventional SILs and water-in-salt (WIS) electrolytes. Furthermore, it demonstrates the successful application of eNMR to highly hydrated SIL systems.

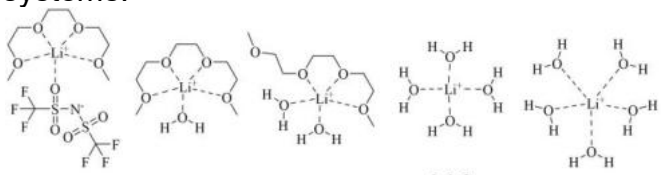

Figure 1: Determined structures via molecular dynamics simulation and presumed structures (*italic*) of a LiTFSI:G3 solution with different amounts of added water.[1]

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Real-Time Multi-Exponential Component Analysis in TD and FFC NMR Relaxometry

Poster: 34

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Fast Field Cycling (FFC) and Time-Domain (TD) NMR relaxometry are widely used to study molecular dynamics in heterogeneous systems such as porous media, polymers, foods, and biological tissues. In many practical cases, longitudinal relaxation cannot be described by a single exponential decay, since different molecular environments contribute distinct relaxation components. Although multi-exponential fitting is well known and routinely applied in analysis, it is often carried out only after the experiment is completed, requiring export of data to external software and repeated manual processing.

During routine FFC-NMR measurements, particularly when acquiring full NMRD profiles, users may recognize only after several hours that additional components are needed or that experimental parameters should have been adjusted. This separation between acquisition and analysis creates a practical bottleneck, increases overall experimental time, and can delay informed scientific decisions.

In this work, multi-exponential fitting is implemented in real time during FFC experiments and high-field, variable-field relaxometry [1] by integrating a flexible fitting engine [2] directly into the acquisition environment of Storm6 platform,
Mono-, bi-, and tri-exponential models, as well as user-defined functions, are supported. At each magnetic field value, the relaxation curve is fitted immediately after acquisition, and the extracted relaxation rates and component weights are updated live to construct the evolving NMRD profile. This allows early identification of multi-component behavior and timely adjustment of experimental parameters when required.

The approach was validated on heterogeneous samples where mono-exponential analysis produced systematic deviations. Real-time visualization reduced post-processing time and supported more efficient experimental workflows. Ongoing work focuses on uncertainty estimation and regularization strategies to further improve robustness of real-time multi-component analysis.

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Poster:

35

FFC-NMR method for acquisition of T1–T2 maps at different relaxation fields.

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Fast Field Cycling (FFC) NMR relaxometry is a powerful technique for probing molecular dynamics through magnetic-field dependent longitudinal relaxation. While conventional FFC measurements provide nuclear magnetic relaxation dispersion (NMRD) profiles and T1 distributions, the characterization of transverse relaxation under field-cycling conditions has been wrongly considered technically limited.

In this work, we present the development of a multidimensional FFC-NMR methodology and demonstrate the capability of generating field-dependent T1–T2 correlation maps, thus extending relaxometric insights into a frequency-resolved multidimensional framework.

The proposed approach combines Fast Field Cycling relaxometry with CPMG-based measurements through dedicated acquisition protocols, enabling the generation of T1–T2 maps at different relaxation fields. The methodology is demonstrated using Parmigiano Reggiano cheese as a representative complex food matrix.

The resulting field-dependent T1–T2 maps provide enhanced characterization of molecular dynamics compared with conventional one-dimensional relaxometry approaches.

The results demonstrate the feasibility of multidimensional FFC NMR T1–T2 relaxation maps experiments and offers additional methods for investigating complex systems in food science, polymers as well as porous materials soft matter.

Data analysis and graphical representation has been done by means of MUpen2D and 'MUpen tool' Software developed by University of Bologna

https://shorturl.at/kXCpW

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Influence of Paramagnetic Relaxation Additives on DNP-enhanced MAS NMR

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In solid-state NMR spectroscopy, dynamic nuclear polarization (DNP) is one of the most prominent methods for generating hyperpolarization in order to enhance sensitivity. DNP is based on the transfer of polarization from the electron spin of a paramagnetic polarization agent (PA) to nuclear spin via hyperfine interaction (HFI). However, paramagnetic relaxation enhancement (PRE) induced by the PA often leads to compromised spectral resolution due to signal quenching of the nuclei close to the PA, giving rise to the occurrence of a 'blind sphere' around the PA. Yet, no quantitative model of paramagnetic relaxation under cryogenic conditions relevant for MAS DNP exists. In order to develop strategies for mitigation of this effect, we want to gain a deeper understanding of paramagnetic relaxation under the conditions typically encountered during MAS DNP NMR. To this end, we investigated the influence that the addition of paramagnetic salts (additives) has on DNP parameters.

We performed MAS DNP measurements of standard DNP formulations (1 M ^{13}C-urea in 60:30:10 d_8-glycerol/H_2O/D_2O with 10 mM AMUPol as PA), to which we added various paramagnetic salts in varying concentrations. Here, we find that the paramagnetic additives lead to a lower steady-state signal enhancement, while the polarization build-up rate was increased. The strength of this effect depends on the spin quantum number *S* of the additive as well as on its concentration, with the tendency of lower spin quantum numbers and higher concentrations leading to a stronger effect. For some additives, also the effect of peak broadening has been evaluated. Our results will aid the development of a quantitative model of paramagnetic relaxation under MAS DNP conditions which is crucial for further developments for site-specific DNP. Furthermore, it provides important information for MAS DNP of paramagnetic (biological) materials, such as heme-containing tissue or blood.

Poster:

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Rotational Resonance for the Selective Boost of Spin Diffusion Pathways under Site-Specific DNP

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In solid-state NMR, dynamic nuclear polarization (DNP) is a versatile hyperpolarization technique with a wide range of applications ranging from structural biology to materials science. However, many large and challenging systems require not only enhanced sensitivity but also site specificity. For this matter, SCREAM-DNP (specific cross-relaxation enhancement by active motions under DNP) allows the selection of site-specific polarization pathways that accumulate hyperpolarization on dynamic groups at cryogenic DNP conditions. The workhorses of SCREAM-DNP are methyl groups that receive polarization from the hyperpolarized ^{1}H network via cross relaxation (CR), and then further propagate it through the ^{13}C network by carbon-carbon spin diffusion (SD).[1]

To fully leverage the potential of SCREAM-DNP, a comprehensive understanding of each polarization transfer step is essential. Following the site-specific CR transfer, this work focuses on the subsequent carbon-carbon SD step. This coherent polarization transfer is mediated by the homonuclear ^{13}C dipolar coupling, enabling the MAS-based recoupling via rotational resonance (R^2) when an integer multiple of the MAS frequency matches the difference in isotropic chemical shifts. Using a model compound, it was found that R^2 recoupling significantly increased the SD rate constant for the n = 1 and 2 conditions. The MAS dependence was then quantified using a broader MAS profile, showing that the spinning frequency strongly affects the SD rate constant.[2] Building on these results, we measured a detailed MAS profile on a different model compound to reveal how stringently the SD buildup must match the R^2 conditions. With the goal of estimating distances through SD rate constants in SCREAM-DNP experiments, we are currently investigating whether the MAS profiles could be used to derive distance information in a manner similar to the R^2-width approach (R^2W).[3] Our findings demonstrate the importance of characterizing the DNP polarization pathways and suggest how a DNP-based experiment could be used to determine important structural parameters.

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Poster:

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Hyperpolarized Xenon as a Quantum Sensor for Dark Matter: The CASPEr-gradient experiment.

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Axions and axion-like particles are well-motivated dark matter candidates that were originally proposed to solve the strong CP problem in quantum chromodynamics and naturally arise in extensions of the Standard Model. If they constitute dark matter, these fields are expected to oscillate coherently at a Compton frequency set by their mass $m_a c^2/\hbar$ and to couple weakly to nuclear spins. The Cosmic Axion Spin Precession Experiment-gradient (CASPEr-gradient) employs precision NMR techniques to search for such interactions over a broad mass range, spanning frequencies from sub-kilohertz up to hundreds of megahertz, using superconducting quantum interference devices (SQUIDs) and tunable LC circuits for signal detection [1, 2].

In this talk, we present the current status of the CASPEr-gradient experiment, including recent commissioning results [1]. A central focus is the development of a xenon delivery scheme that combines long nuclear spin relaxation times with strongly enhanced spin polarization achieved via spin-exchange optical pumping, together with high spin densities enabled by the moderate liquefaction temperature of xenon. We aim to produce large amounts of hyperpolarized liquid ^{129}Xe, typically 0.5 mL to 1.5 mL every 15 min to 30 min, in continuous flow. These developments lead to significant enhancements in signal strength and experimental sensitivity and represent an important step toward extending the reach of CASPEr-gradient into previously unexplored regions of axion and axion-like particle parameter space.

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Poster:
39

Liquefaction of hyperpolarised xenon for dark matter searches

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The Cosmic Axion Spin Experiment – Gradient (CASPEr-Gradient), part of the international CASPEr collaboration, searches for signatures of axions and axion-like particles (ALPs), hypothetical particles that could constitute dark matter, by probing their coupling to nuclear spins using nuclear magnetic resonance (NMR) techniques [1]. An oscillating axion/ALP field may resonantly drive nuclear spin precession in a sample placed in a static magnetic field, and the resulting precessing magnetization may be detected by sensitive magnetometers. The experimental sensitivity depends on the polarization of the sample. Therefore, in CASPEr-Gradient, we aim to use ~ 2 mL of liquid hyperpolarised xenon (HP-^{129}Xe) [2].

We present the transport, compression, and liquefaction of HP-^{129}Xe produced using the spin-exchange optical pumping (SEOP) technique, along with the latest updates and NMR spectra of ^{129}Xe near its triple point. The experimental scheme is as follows: ~ 1.5 L of HP-^{129}Xe gas is transported from the SEOP setup to the detection setup using a pneumatic compressor. The temperature of the sample holder in the detection setup is regulated by a flow of nitrogen gas and is maintained at ~ 170 K. The pressure of the HP-^{129}Xe is increased above its saturation vapor pressure by compression, leading to its liquefaction in the sample holder within a few minutes. The relaxation times of HP-^{129}Xe in the compressor and the detection setup are of crucial importance and are being investigated, along with polarization conservation during liquefaction.

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Investigating Parahydrogen-Induced Hyperpolarization and Solidification of Biocompatible Molecules

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Parahydrogen-induced hyperpolarization offers a rapid and cost-effective route to generate highly polarized molecular probes for NMR and MRI applications.[1] Purification by solidification is an attractive way to isolate such molecules for biomedical applications.[2] In this work, SLIC-SABRE and DRF-SLIC pulse sequences were optimized for nicotinamide, yielding up to 12% ^{15}N polarization in 100 mM nicotinamide at natural abundance in methanol-d_4.[3] The hyperpolarization survived ^{15}N protonation with HCl, forming the corresponding soluble nicotinamide hydrochloride salt. However, subsequent precipitation with diethyl ether resulted in a complete loss of the ^{15}N polarization.

Building on previous work within our group, where ^{13}C polarization in hyperpolarized [1-^{13}C]fumarate was successfully retained during acid-based precipitation, the present study investigates the molecular factors governing whether polarization is preserved during liquid-solid phase transitions. Sodium pyruvate was selected as a second model system due to its biocompatibility, ionic carboxylate functionality, and established SABRE hyperpolarization pathway.[4] In contrast to nicotinamide, where polarization resides on an aromatic ^{15}N nucleus, pyruvate carries polarization on the carboxylate ^{13}C nucleus and shares this structural feature with fumarate. Hyperpolarization conditions for pyruvate were optimized and a series of experiments were performed using different physicochemical methods to precipitate the hyperpolarized pyruvate. In contrast to fumarate, hyperpolarized pyruvate lost its ^{13}C polarization upon precipitation in all cases.

The contrasting behaviour of fumarate, pyruvate, and nicotinamide suggests that neither salt formation nor the presence of a carboxylate functionality alone is sufficient to preserve hyperpolarization during solidification. This work aims to identify the molecular and spin-dynamical factors responsible for polarization retention.

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Poster:

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Sensitivity enhanced solid-state NMR investigations on multi-layered adsorbents

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Cellulose-based functionalized adsorbents find application in a variety of fields, including chromatography, drug loading and protein immobilization. The cellulose core functions as an efficient, and environmentally friendly support base for a wide variety of materials. In an ongoing collaboration with the Fraunhofer Institute for Cell Therapy and Immunology (IZI), we are investigating an adsorbent comprising a polydopamine (PDA) and a lysine layer. The outer lysin layer of the adsorbent is capable of binding the $A\beta_{1\text{-}42}$ protein which plays a significant role in the development of Alzheimer 's disease.

A range of cellulose beads was selected for comparison in order to determine the most suitable adsorbent for NMR and DNP investigations. The unmodified adsorbent was utilized as a reference compound in order to compare the benefits of incipient wetness impregnation (IWI) [1] and matrix-free (MF) [2] preparation of DNP samples. Isotope-enriched material was used to investigate the inter- layer interactions using 2D experiments. Multiple variations of the synthesis were compared using natural abundance material, with an emphasis on the build-up time (T_B) of the samples. Advanced fitting mechanisms were explored to achieve accurate determinations of T_B. ATR-IR and liquid-state NMR were utilized to supplement the investigations.

A clear correlation was observed between the size of the cellulose beads and the relaxation time. Samples prepared using IWI demonstrated a clear trend of superior enhancement, while MF preparations exhibited enhanced resolution. The effects of different levels of rehydration on the MF samples were investigated, achieving mixed results. A loss of the PDA layer was observed during subsequent reaction steps. In addition, we investigated alternative synthesis pathways encompassing either copolymerization or the utilization of rocking shakers during synthesis. Both approaches yielded noticeably increased build-up times on the samples, suggesting a desired increase in shell layer size. Furthermore, a recurring and unexpected reduction in build-up time was identified subsequent to the addition of the Aβ protein.

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Poster:

42

Following ^{1}H Spin Polarization across Phase Transitions

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Parahydrogen-induced polarization (PHIP) is an effective way of enhancing NMR signals, typically several orders of magnitude higher than thermal equilibrium, but it polarizes only molecules that are directly involved in the hydrogenation reaction. In solution, polarization transfer between molecules requires either molecular diffusion to enable intermolecular Spin Polarization-Induced NOE (SPINOE) [1] which can be weak, or polarization transfer through intramolecular J-couplings to a labile proton followed by rapid proton chemical exchange (PHIP-X).[2] However, in solid-state, nuclear polarization can propagate via dipolar-coupled spin networks through spin diffusion, providing a molecular diffusion- and exchange-independent route for polarization transfer to other molecules. Combining PHIP with solid-state spin diffusion (PHIP-SSD) offers a strategy to transfer polarization from hyperpolarized source molecules to non-polarized target molecules. While PHIP-SSD has previously been demonstrated for ^{13}C nuclei,[3] its potential for ^{1}H spins remain largely unexplored. In this work, we investigate whether ^{1}H hyperpolarization survives liquid–solid–liquid phase transitions, how different precipitation conditions can influence ^{1}H and ^{13}C polarization, and whether ^{1}H polarization can be transferred to neighbouring molecules.

In our experiments, [1-^{13}C]fumarate (at natural isotopic ^{13}C abundance) was produced via trans-hydrogenation of acetylene dicarboxylic acid using parahydrogen [4], with fumarate's two ^{1}H nuclei initially in a singlet state. An adiabatic SLIC sequence converts this singlet order into observable ^{1}H and ^{13}C magnetization, respectively [5]. Crystallization was performed in a 400 mT Halbach magnet by adding acids (DCl or D_2SO_4) to the reaction mixture followed by redissolution in alkaline D_2O [6]. We obtained 43% polarization on ^{13}C before crystallization, and up to 26% after redissolving. Further, we obtained 38% ^{1}H polarization on [1-^{13}C]fumarate before crystallization. After redissolving, the remaining ^{1}H polarization was only 0.5%. We performed a series of ^{1}H T_1 measurements of solution- and solid-state fumarate, and were able to confirm that the ^{1}H polarization is lost during the liquid-solid phase transition, and not due to short T_1 in either the solution or solid state. We are now performing direct NMR measurements of these precipitation processes to understand what is driving the loss of ^{1}H polarization.

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Poster:

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Solid-State NMR measurement of Spin Diffusion and Relaxation for PHIP-Polarized Solids

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Parahydrogen-induced polarization (PHIP) is an efficient method to generate nuclear hyperpolarization. However, its applicability is limited, since only molecules that directly participate in parahydrogen-based reactions can be polarized. Recently, approaches combining PHIP with solid-state spin diffusion (PHIP-SSD) have been introduced to transfer polarization from a PHIP-active precursor to other molecules in the solid state. This approach could provide an inexpensive route to hyperpolarize a wide range of molecules.
Here, we used solid-state NMR relaxation and spin diffusion measurements to explore how the solid-state environment influences polarization transport in PHIP-derived solids. Precursor systems were precipitated under controlled conditions, and we investigated different drying protocols, sample deuteration fractions, and temperatures. We observe pronounced differences in relaxation times depending on the sample preparation parameters. The ^{1}H T_1 values are largely independent of the precipitation acid (HCl vs H_2SO_4) and drying conditions, whereas the ^{13}C T_1 values differ strongly between protonated and deuterated samples, with protonated samples exhibiting much longer relaxation times (~200 s) compared to deuterated samples (~12 s). Our results suggest that polarization transport in PHIP-derived solids is governed by an interplay between spin diffusion and relaxation processes. High-field solid-state NMR measurements provide insight into relaxation processes that influence spin diffusion in these systems. These findings highlight the importance of sample preparation conditions for optimizing polarization transfer in PHIP-SSD hyperpolarization experiments.

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Poster:

44

Effect of subsegmental dynamics of PEG on NMR observables

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Classically, the conformational dynamics of polymer melts and solution is fudged into the Kuhn length, and the solvent-polymer interaction is described with the χ mean-field parameter and a scaling exponent. Especially interesting is the case of good solvents where the scaling exponent is similar and any differences originating from sub-Kuhn segment level is expected to be minimal. However, we have recently observed that the effect of solvent on Residual Dipolar Coupling (RDC) arising from the network constraint in model 4arm polyethylene glycol (PEG) networks can be significant and simple solvent quality argument within Flory-Rehner theory may not be sufficient to explain the results [1,2].

^{13}C spectra and time-domain ^{1}H multiple-quantum NMR data supplemented by atomistic molecular dynamics simulation are used to try to understand the differences in the PEG-water and PEG-toluene systems. On the one hand, ^{13}C single-pulse spectra in solution state (relaxed end-to-end distances) show that the methylene peak in water is significantly downfield compared to toluene, which can be correlated with differences in the dihedral angle distribution especially the higher population on trans C-O-C-C bond. On the other hand, MQNMR data of networks measured at same swelling ratio highlights variations in the RDC arising from different dihedral dynamics within the Kuhn segment. These observables are correlated with parameters obtained from simulations such as bond and dihedral angle distributions and the orientation autocorrelation function of proton-proton and carbon-carbon internuclear vectors.

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Poster:
45

Multi-Stimuli Responsive Supramolecular Systems Studied by NMR Spectroscopy

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As one of the most impactful analytical techniques in modern chemistry, NMR spectroscopy is indispensable not only for molecular characterization but also for investigating a wide range of molecular properties. The combination of one- and two-dimensional NMR techniques provides a powerful approach for the characterization of supramolecular structures and their dynamic behavior.
This work demonstrates the application of NMR for the investigation of a multi-stimuli-responsive supramolecular system based on pyridine-oligo(phenylene ethynylene) (Py-OPE) molecules, which incorporate both acid- and light-responsive units. Light irradiation of the Py-OPE-based molecules produces highly stable states with high *E*/*Z* ratios, while protonation of the pyridine unit alters the energetic landscape sufficiently to enable back-switching using the same wavelength. Subsequent deprotonation enables the system to reset to its initial state. Using a self-built in situ irradiation setup, the photoisomerization process of the molecule was investigated, and the quantum yield was determined. The results show, that due to their large conjugated π-system, go beyond simple adaptability to external stimuli, demonstrating an elementary form of molecular memory.
Additionally, the molecules exhibit aggregation behavior with increasing concentration. To further elucidate this behavior and its influence on the controllable states of the system, the supramolecular polymerization of a slightly modified Py-OPE molecule was investigated in the absence and presence of sulfonic acids. Characterization by one- and two-dimensional NMR techniques, complemented by DFT calculations, revealed substantially different supramolecular structures depending on the presence of acid and highlighted the role of the anions during the aggregation process. These findings provide further insight into the supramolecular processes underlying the controllable states of the system and enable a step towards unravelling the concept of molecular memory.

Poster:
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Sidechain-Backbone Connectivity Revealed by Sensitivity Enhanced Time-Shared NMR Spectroscopy

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NMR has become a solid method to study biomolecules such as proteins and nucleic acids. NMR data can be used to calculate structure of proteins, identify key interactions in enzymatic activities and obtaining the dynamics profile in large complexes. However, size is a limiting factor in NMR experiments. Large proteins and molecular complexes consist of multiple spins, all of which have chemical shifts that have a finite range. Large proteins tend to have crowded spectra with high spectral congestion, which are impractical for high-resolution work. This problem can be tackled by using high-dimensionality NMR. By adding more dimensions to the NMR spectra, a better peak-separation can be achieved, leading to spectra that can be more easily assigned and interpreted. However, high-dimensionality comes with a cost. The addition of dimensions inevitably increases the experimental time, relaxation effects decrease the sensitivity as the sequences get longer, and inefficient mixing schemes cause an accumulated loss of magnetisation during the transfer process.

In this work, we tackle this problem by designing and testing mixing schemes to enhance the sensitivity of 4D and 5D experiments. The designing process includes usage of optimal control pulses to enhance the sensitivity of the indirect dimensions. We also develop multi-dimensional experiments that can link amino acids in proteins and sidechains of different residues. Such information is crucial for structure calculations, and can provide important insights for biological mechanisms and functions. To achieve that, we are using proton-proton dipolar-interaction-based mixing schemes and optimise them to obtain high sensitivity multi-dimensional NMR spectra. We also design time-shared experiments to obtain information about the backbone and the sidechains connectivity simultaneously with high resolution and sensitivity.

Poster:

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Effects of Microwave Irradiation on Gadolinium doped Bismuth Oxido Nanoclusters in Solid State NMR

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The use of polynuclear bismuth oxido nanoclusters has been of interest in various fields, including their use in drugs to treat gastrointestinal diseases and in the photocatalytic decomposition of organic pollutants in aqueous solution.[1,2] They have also been used in the synthesis of thin films made from nanoscale β-Bi_2O_3.[3] Specifically, those of size $\{Bi_{38}O_{45}\}$ are of significance, since these make up the majority of the reported structures.[4] Recently, there has been growing interest in doping these clusters with paramagnetic ions, especially with those in the lanthanide series (e.g. Gd^{3+}, Tb^{3+}, Eu^{3+}), as well as Mn^{2+}.[5] Clusters doped with Mn^{2+} and Gd^{3+} are of particular interest, due to their potential uses as Polarization Agents (PA) in Solid Effect (SE) Dynamic Nuclear Polarization (DNP) enhanced Magic Angle Spinning (MAS) NMR.[6] Preliminary studies have already shown their feasibility for this use.[5]
Here, we present a more systematic study of these clusters with different surface modifications. We have used alanine, phenylalanine and methacrylate with different isotopic labeling, both with approximately 1 w% Gd^{3+} doping and without. These studies revealed two interesting phenomena, on the one hand very fast T_1 times were observed for both protons and carbon, without paramagnetic dopants. On the other hand, we observed interesting thermal effects, indicating an interaction between the Bi and the microwaves. Measurement of the ^{79}Br T_1 times of KBr revealed a broad temperature distribution within the sample at an external temperature of 103 K and a MAS frequency of 7 kHz.[7]

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3D Printing for Applications in Solid State NMR

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Additive manufacturing, to be more precise 3D printing, enables custom, low-cost and reproducible hardware for solid state nuclear magnetic resonance (NMR) spectroscopy. The present work highlights specific operational areas where 3D-printed components have been developed and applied to extend experimental capabilities:

a) Stable Magic Angle Spinning: Low-cost 3D-printed parts were developed to achieve stable magic angle spinning of several kHz for different rotor diameters and types, providing not only low-cost alternative to commercial probehead components[1,2], but also for specific scenarios like quantitative MAS NMR; single-crystal and NMR and toxic NMR.[3]

b) Chemical Exchange in Unstable Emulsions: Specialized 3D-printed hardware to enable active mixing during NMR measurements for investigation of unstable emulsions, facilitating studies of chemical exchange between interfaces.[4]

These results demonstrate how additive manufacturing opens pathways for the development of new NMR instrumentation.

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Poster:

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Advanced Methods and Applications in 1D and 2D Low-Field NMR Spectroscopy

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Low-field (benchtop) NMR spectroscopy has gained increasing attention as a versatile analytical tool due to its compact design, low operating costs, and easier integration with other analytical techniques. However, compared to high-field instruments, reduced spectral resolution and lower sensitivity require dedicated optimization of pulse sequences, acquisition parameters, and data processing protocols.[1-5]
In this work, we demonstrate three advanced methodologies and their applications in low-field NMR spectroscopy at 80 and 90 MHz.
The first part covers HPLC-NMR, which combines chromatographic separation with spectroscopic characterization. While chromatography enables the separation of analytes according to molecular size (SEC), particularly relevant for polymer analysis, or polarity (LAC), especially suited for small molecules, NMR spectroscopy provides structural information for each separated component. Such benchtop HPLC-NMR methodologies have been developed in our group for more than a decade and have recently been extended from one-dimensional ^{1}H NMR to two-dimensional experiments, including COSY and HSQC, to improve spectral resolution and structural elucidation further.[1-3]
The second topic compares different solvent suppression techniques and their applicability across various experimental setups, such as static or flow NMR.[4] Efficient solvent suppression is particularly important for reaction monitoring and HPLC-NMR experiments, where using large amounts of deuterated solvents is often impractical.
Finally, we present the determination of polymer molar masses by DOSY-NMR. Unlike conventional SEC methods, DOSY requires no chromatographic separation columns, reduces solvent consumption, and provides additional spectroscopic information. A pulsed-field-gradient method was implemented for the determination of molar masses up to 1000 kg·mol^{-1} within 11 min. Furthermore, molar-mass distributions and chemical composition profiles can be obtained with this method.[5]

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Poster:

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Broadband Benchtop NMR Spectroscopy for Research and Industrial Applications

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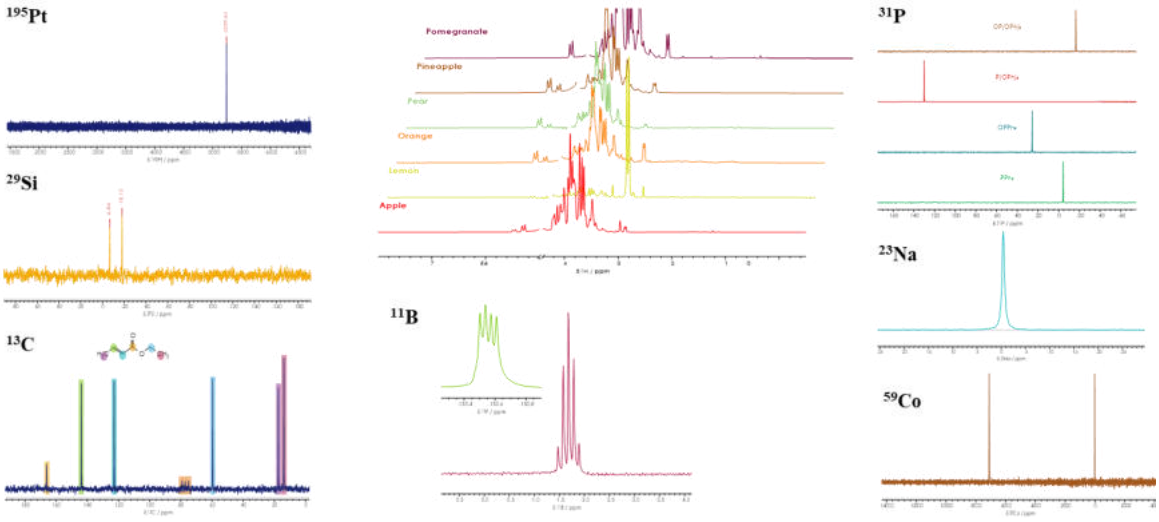
The X-Pulse 90 is a benchtop NMR spectrometer built around a 90 MHz permanent magnet. It combines advanced features typically associated with high-field systems with the simplicity and user-friendly design of a compact instrument. With full broadband capability, adjustable temperature control, and automated operation, the X-Pulse provides both flexibility and precision across a wide range of NMR applications. In this work, we demonstrate the performance of the X-Pulse system in several analytical contexts, including the suppression of undesired signals using a range of solvent suppression sequences. This capability is illustrated using different batches of fruit juice samples prepared in buffer solution, in which the dominant water signal is effectively suppressed. As a result, signal overlap is reduced, enabling improved quantification of key components such as organic acids and sugars. The suppression sequences can also be extended to target multiple residual signals, offering enhanced flexibility for diverse analytical challenges.

In addition, the X-Pulse is well-suited for real-time reaction monitoring due to its fully tuneable broadband capability, making it applicable across a wide variety of reaction types. When combined with flowNMR and an external lock, the system enables the acquisition of quantitative kinetic and mechanistic data, providing insight into reaction pathways and catalytic efficiency. Furthermore, the instrument operates over a broad temperature range (0–60°C), allowing investigation of dynamic processes and the determination of thermodynamic and kinetic parameters.



Towards a Compact NV Relaxometry Demonstrator for Clinical EPR Applications

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Conventional Electron Paramagnetic Resonance (EPR) spectroscopy can be used to detect clinically relevant biological radicals such as reactive oxygen species [1], which are indicators for several human diseases. However, the widespread clinical integration is hindered by spectrometer size, the need for relatively high external magnetic fields and concentration sensitivity limited to approximately 10nM/$\sqrt{\text{Hz}}$ [2].
Nitrogen-vacancy (NV) centers in diamond are a highly promising candidate to resolve these issues. Using optically detected magnetic resonance techniques at ambient temperature without high external magnetic fields, these quantum sensors allow single electron spins to be detected [3] and have even enabled SARS-CoV-2 RNA identification [4]. While the detection of a small number of spins is feasible, achieving low concentration detection limits in liquid environments remains challenging for NV relaxometry. To address this, chemically functionalized nanodiamonds hosting NV centers [5] will be used to selectively bind target molecules, thereby increasing local concentration and enhancing detection sensitivity.
The aim of this work is to develop a compact and cost-effective demonstrator for NV relaxometry measurements on biological samples tailored for future clinical applications. Building upon pioneering work in EPR spectrometer miniaturization by the Institute of Smart Sensors [6], the setup will incorporate custom application-specific integrated circuits for both microwave excitation and optical readout of NV centers. The latest progress towards this goal and future perspectives will be presented.

Literature:

[1] B. Fink et al., Int. J. Mol. Sci. 2025, 26, 5209
[2] G. R. Eaton et al., Springer 2010
[3] F. Shi et al., Science 2015, 347, 1135
[4] C. Li et al., Nano Lett. 2022, 22, 43
[5] A. Sadzak et al., Mater. Quantum. Technol. 2025, 5, 013001
[6] H. Lotfi et al., IEEE J. Solid-State Circuits 2024, 59, 1421

Poster:

52

A 500 mT Lightweight Nested Halbach Magnet with 10 ppm Homogeneity for Portable NMR

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Maximiliane Waldecker, University of Stuttgart, Pfaffenwaldring 47, 70569 Stuttgart/DE

Halbach magnets provide a compact and energy-efficient approach for generating highly homogeneous magnetic fields in portable NMR systems. Building upon the design concepts introduced by Raich and Blümler [1] and recent optimization strategies for multilayer Halbach arrays [2], this work presents a lightweight nested Halbach magnet targeting a magnetic field strength of approximately 500 mT with a field homogeneity better than 10 ppm over the sensitive volume. The proposed design combines high magnetic performance with low weight, low material cost, and compatibility with additive manufacturing. The magnet consists of three nested Halbach rings, each comprising two axially separated layers. The support structure is fabricated by stereolithographic (SLA) 3D printing, enabling high mechanical accuracy while minimizing weight. The magnet design independently addresses the two dominant sources of field inhomogeneity. Edge effects are compensated by optimizing the axial spacing between the Halbach layers according to the theoretical framework presented in [1,2]. Besides significantly improving field homogeneity, this optimization also increases the magnetic field generated by the outermost ring. The remaining discretization-induced field distortions are compensated using locally integrated inserts fabricated from a custom soft-magnetic resin-iron powder composite. The effective permeability of this composite is tailored while accounting for demagnetization effects following the model of Lin *et al.* [3]. The composite is injected into dedicated cavities integrated into the 3D-printed support, enabling application-specific passive shimming without increasing the overall magnet weight. As a first proof of concept, a prototype consisting of three nested single-layer Halbach rings was fabricated and experimentally characterized. Hall probe measurements agree with finite-element simulations within 1 %, validating the electromagnetic design methodology and the mechanical manufacturing concept. The measured field homogeneity already enables reproducible NMR measurements. The complete two-layer nested Halbach magnet incorporating the passive shimming approach is currently under construction and is expected to achieve the targeted field strength of 500 mT with a homogeneity better than 10 ppm.

Literature:

[1] P. Blümler and H. Soltner, Appl. Mag. Res. 2023, vol. 54, no. 11–12.
[2] P. Yu *et al.*, J. Mag. Res., vol. 344, p. 107322, 2022.
[3] G. Q. Lin, Z. W. Li, L. Chen, Y. P. Wu, and C. K. Ong, J. Magn. Magn. Mater., vol. 305, no. 2, pp. 291–295, 2006.

Poster:

53

Fast Field Cycling Relaxometry: From Molecular Dynamics to Industrial Applications

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Keywords: theory and methods, instrumentation, Fast Field Cycling NMR.

Fast Field Cycling NMR Relaxometry (FFC NMR) is a powerful NMR technique that enables the measurement of longitudinal relaxation times (T_1) over a broad range of magnetic fields, spanning several orders of magnitude without changing the spectrometer frequency. The resulting Nuclear Magnetic Relaxation Dispersion (NMRD) profiles provide valuable insights into molecular dynamics by probing motion over a wide range of correlation times.
In particular, access to low Larmor frequencies allows the investigation of slow molecular processes, including surface dynamics, collective motions, and intermolecular interactions, which are often difficult to characterize using conventional spectroscopic techniques. Because radiofrequency radiation can penetrate a wide variety of materials, FFC NMR is particularly suited to heterogeneous and complex systems, including liquids, solids, gels, and aggregated materials.
In this work, recent developments in FFC NMR are presented together with selected applications demonstrating its potential as a tool for structural and dynamic characterization. NMRD profiles are used to investigate molecular mobility, identify weak intermolecular interactions, and provide qualitative and quantitative information on the structure and dynamics of complex materials.
Beyond its value as a fundamental research technique, these capabilities highlight the potential of FFC NMR for practical applications in material characterization, quality assessment, and off-line process monitoring. The development of advanced FFC NMR instrumentation and methodologies represents an important step toward transferring NMR relaxometry from a predominantly research-oriented technique to a more accessible and versatile industrial analytical tool.

References

[1] Ferrante and Sykora Adv. Inorg.Chem. Vol. 57, p. 405.
[2] R. Kimmich and E. Anoardo Progress in Nuclear Magnetic Resonance Spectroscopy44 (2004) 257-320
[3] D. Kruk, R. Meier, and E. A. Rossler PHYSICAL REVIEW E 85, 020201 (R) (2012)

Philosophicum - FGMR floor map

Georg-Forster building
(cafeteria &
vending machines for beverages)

mensa card
vending machine

to cafeteria
„*insgrüne*“

Lecture Halls Philosophicum EG:

Plenary + Parallel: P1
Parallel: P2 - P3

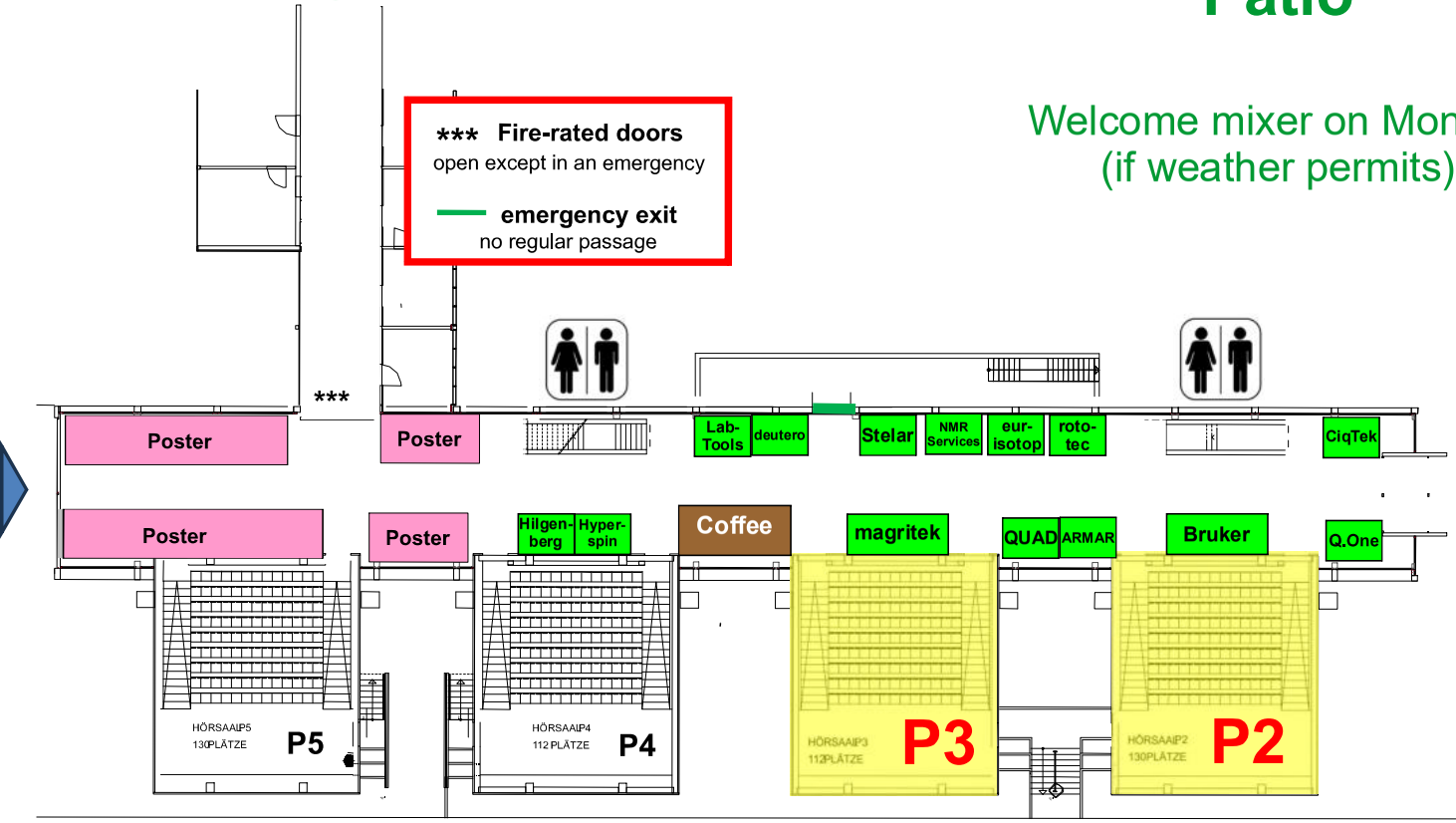
Foyer P2-P5:
Posters + vendors

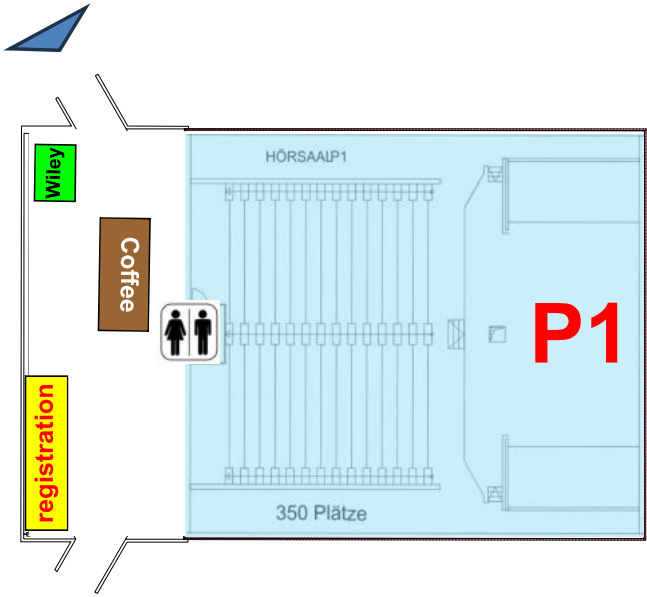
Patio

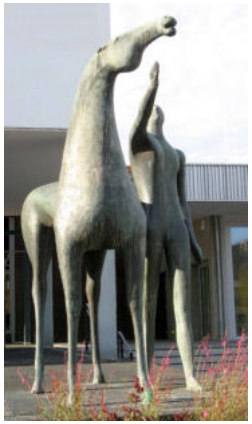
Welcome mixer on Monday
(if weather permits)

*** **Fire-rated doors**
open except in an emergency

emergency exit
no regular passage







PHILOSOPHICUM

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

ERDGESCHOSS
GROUNDFLOOR

- Cafeteria / Cafeteria
- Poststelle / Mailroom
- Briefkasten / Mailbox
- Information / Hausmeister / Information / Janitor
- Aufzug / Elevator
- Kopierer / Photocopier
- Barrierefreier Zugang / Barrier-free access
- Wickeltisch / Diaper-changing table
- Stillraum / Breast-feed room
- Standort / Location
- Hörsäle / Lecture halls
- Dekanat FB05 / Dean's office faculty 05
- Institute / Fächer / Seminars / Departments
- Fakultätssaal / Faculty hall
- Verwaltungsgebäude / Administration building
- Schule des Sehens / School of Seeing
- Bereichsbibliothek Philosophicum / Libraries
  1. Standort Mittlere und Neuere Geschichte / Library of Medieval and Modern History
  2. Standort Slavistik / Osteuropäische Geschichte I / Library Slavic Studies Eastern European History I
  3. Standort Philosophie / Library Philosophy

Hörsaal P2 / Lecture hall P2
Hörsaal P3 / Lecture hall P3
Hörsaal P4 / Lecture hall P4
Hörsaal P5 / Lecture hall P5
1.OG Fakultätssaal Faculty hall
WC
UG
Schule des Sehens / School of Seeing
Hörsaal P1 / Lecture hall P1
Aufgang zu IKM-Abteilung Musikwissenschaft und zur Bibliothek Musikwissenschaft 1. OG / Access to Department of Musicology and Library of Musicology
Aufgang zum Fakultätssaal 1. OG / Access to Faculty Hall
Eltern Kind Raum / Parent-child room
Haupteingang / Main entrance
Hörsaal P6 / Lecture hall P6
Hörsaal P7 / Lecture hall P7
Hörsaal P10 / Lecture hall P10
Hörsaal P11 / Lecture hall P11
Hörsaal P12 / Lecture hall P12
Hörsaal P13 / Lecture hall P13
Hörsaal P15 / Lecture hall P15
Übergang zum Georg Forster-Gebäude und Bibliothek Access to the Georg Forster-Building and Libraries
Zugang Bereichsbibliothek / Institute / Fächer Access to the Libraries / Seminars / Departments
Philosophisches Seminar / Department of Philosophy
Innenhof / Courtyard
Innenhof / Courtyard
Innenhof / Courtyard
Historisches Seminar / History Department
Philosophisches Seminar / Department of Philosophy
Institut für Slavistik / Department Slavic Studies
Historisches Seminar / History Department

47. FGMR Discussion Meeting 2026

Location Plan Campus

GESELLSCHAFT DEUTSCHER CHEMIKER

registration/conference

- conference
- ATM
- food
- bus/tram stop

Tram stop UNIVERSITÄT
Tram stop PFEIFFER WEG
Universität
Downtown
Footpath to the university campus
Bakery
Forum
Baron
Qkaff
Alte Mensa
Albert-Schweitzer-Straße
Johannes-v.-Müller-Weg
Philosophicum
Georg Forster-Gebäude
ReWi
Jakob-Welder-Weg
alte Chemie
Johann-Joachim-Becher-Weg
C.-Kleinmann-Weg
SB II
Naturwiss. Fakultätsgeb.
Muschel
Diwan
Anselm-Franz-von-Bentzel-Weg
Grüne Schule
Botanischer Garten
Gymnastik u.Schwimm-
Sport
Botanischer Garten
Große Sporthalle
Stadion
Hanns-Dieter-Hüsch-Weg
Dalheimer-Weg
Backhaushohl
Beachvolleyball/ Basketballanlage
Rasensportanlage
Bogenschießanlage
Tennisanlage
Neubau Kita
Technisches Betriebszentrum
Entrance main gate
Ackermannweg
Lucy-Hillebrand-Straße
Koblenzer Straße
Max-Planck-Institut für Polymerforschung MPI-P
Institut für Molekulare Biologie
Neubau Biologie 2.BA
Neubau Biologie 1.BA
Hahn-Meitner-Weg
Max-Planck-Institut für Chemie MPI-C
Duesbergweg
Schulz-Horner Geb.
Physics
Mainzer Mikrotron MAMI
Staudingerweg
Helmholtz-Institut
Nuclear Physics
Physikalische Chemie (Neubau)
Chemie
Mensa
Studierenden-werk
Hochschule für Musik
Biochemie Genetik
Nuclear Chemistry
F.-v.-Pfeiffer-Weg
F.-Strassmannweg
Saarstraße
Wittichweg
Friedrich-von-Pfeiffer-Weg
Gonsenheim
Autobahn
Koblenzer Str. / HDI-Gerling
Bretzenheim / Lerchenberg
N
0 m
100 m
200 m

47. fgmr

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Getting from Frankfurt Airport to Mainz – September 13/14

Please note: Due to construction work, the regular **S8 train between Frankfurt Airport and Mainz may not be running on September 13 and possibly also on September 14**.

At the moment, it looks as if the main problems will occur over the weekend and that public transportation from the airport to Mainz should be operating normally again on Monday. However, the information provided by Deutsche Bahn is somewhat contradictory at the moment — sorry!

As the situation may be different on Sunday and Monday, the first thing to do is to check whether trains to Mainz are running.

You can check the current departures on the webpage https://www.bahnhof.de/en . Select the station "Frankfurt (Main) Flughafen Regionalbahnhof" and then click on "Live Departures / Arrivals." (the link above should do this automatically)

If you see an **S8 to Wiesbaden Hbf**, you can take that train. Tickets can be purchased from the ticket vending machines in the station.

If no S8 train is running:

The easiest option is to take the **S8X replacement bus** from Frankfurt Airport to Mainz Hauptbahnhof (Mainz Central Station).

If you arrive by plane:

1. After collecting your luggage, follow the signs for "Long-distance trains / Fernbahnhof" and The Squaire.
2. You do not need to go to the Regional Train Station for the replacement bus.
3. The S8X replacement bus departs from the area around The Squaire / Frankfurt Airport Long-distance Train Station ("Am Squaire").
4. Take the S8X towards Mainz Hauptbahnhof.
5. From Mainz Hauptbahnhof, continue as described in the General Information section of the Conference Program.

Arriving by train

If you arrive at Frankfurt Airport Long-distance Train Station (Fernbahnhof):

This is actually very convenient. The Fernbahnhof is located directly underneath The Squaire. Simply follow the signs from the station towards The Squaire / Am Squaire and look for the S8X replacement bus to Mainz.

Important: If the S8 is not running, do not look for the normal S8 at the Regional Train Station. Follow the signs to The Squaire / Fernbahnhof for the replacement bus instead.

If you are unsure where to go, ask airport staff for:

"S8X replacement bus to Mainz Hauptbahnhof / Schienenersatzverkehr nach Mainz."

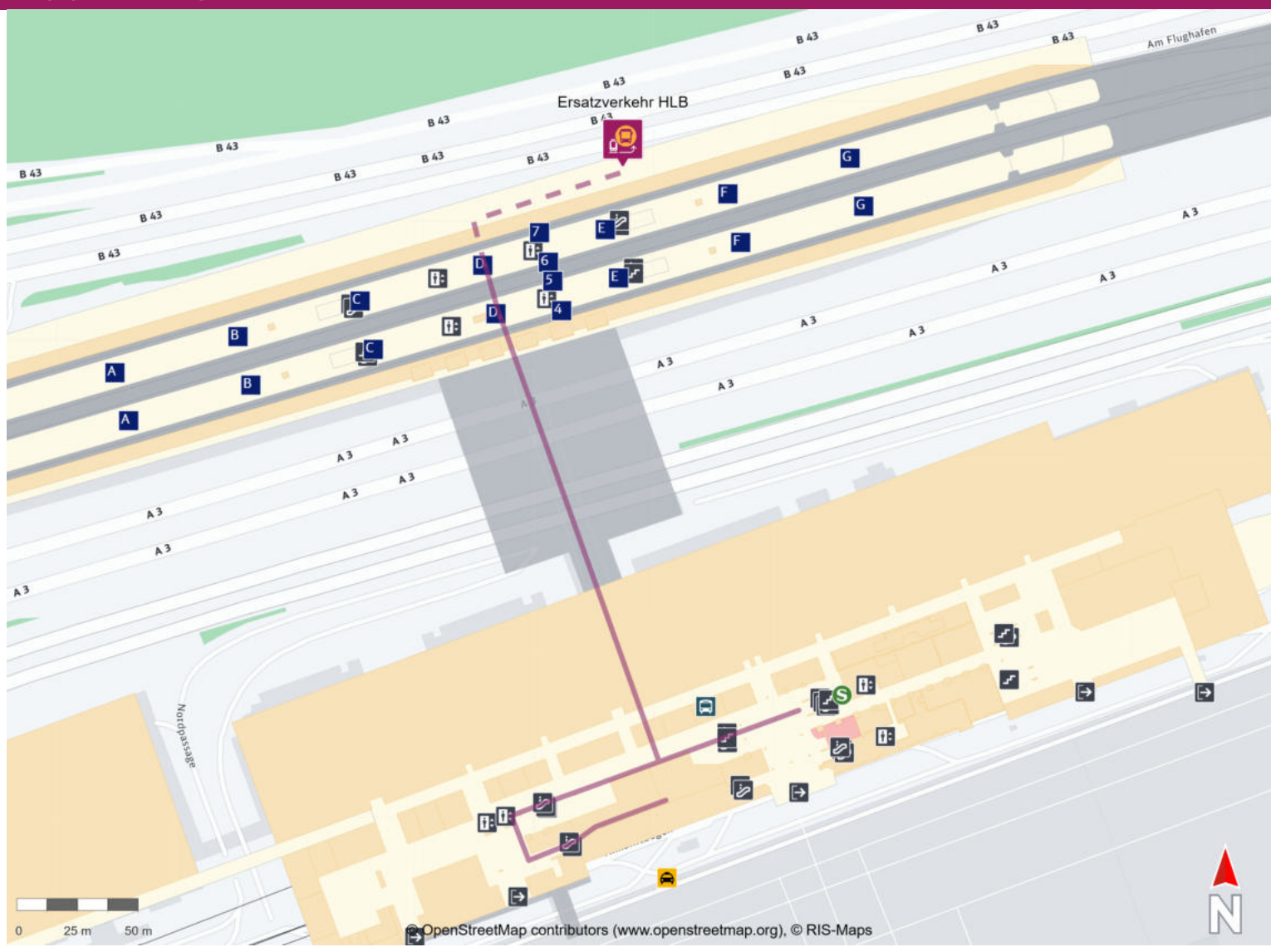
(attention: a taxi will cost 75€ one way!!)

Ihr Weg zum Ersatzverkehr
Frankfurt (Main) ✈ Flughafen Regionalbahnhof

Your way to the replacement service stop Frankfurt (Main) ✈ Flughafen Regionalbahnhof

Abfahrtszeiten und weitere Informationen

Departure times and additional information



Barrierefreier Weg
Accessible way

Nicht-barrierefreier Weg
Non-accessible way

Wegbeschreibung zur Ersatzhaltestelle*

Verlassen Sie den Bahnsteig und begeben Sie sich zwei Ebenen nach oben. Überqueren Sie den Übergang zum Fernbahnhof und nehmen Sie den Ausgang neben der DB Information. Die Haltestelle befindet sich rechts des Ausgangs.

*Directions to the replacement service stop**

Leave the platform and go up two levels. Cross the crossing to the long-distance station and take the exit next to the DB Information. The bus stop is to the right of the exit.

Kontakt/Contact:

Internet bahnhof.de/frankfurt-main-flughafen-regionalbahnhof

* Eine Fahrradmitnahme im Ersatzverkehr ist grundsätzlich nicht möglich.
Taking bicycles on replacement services is generally not possible.