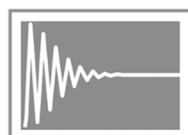


# 44<sup>th</sup> FGMR Annual Discussion Meeting 2023

Annual Discussion Meeting of the Magnetic Resonance Division  
of the German Chemical Society

18 – 21 September 2023, University of Konstanz, Germany

Conference Programme



## Programme

### Overview

Programme Overview - 44th FGMR Annual Discussion Meeting 2023, Konstanz			
18-21 September 2023			
Monday, 18 Sep	Tuesday, 19 Sep	Wednesday, 20 Sep	Thursday, 21 Sep
	<b>Plenary Session 1</b> 08:30 - 10:30 R712	<b>Plenary Session 3</b> 08:30 - 10:30 R712	<b>Plenary Session 5</b> 08:30 - 10:30 R712
	Coffee break 10:30-11:00	Coffee break 10:30-11:00	Coffee break 10:30-11:00
<b>JEOL user meeting</b> 9:30-12:30 M630	<b>Parallel Sessions 1</b> 11:00 - 12:00 Session A R711 Session B R611 Session C R513	<b>Parallel Sessions 3</b> 11:00 - 12:00 Session A R711 Session B R611 Session C R513	<b>Parallel Sessions 5</b> 11:00 - 11:40 Session A R711 Session B R611 Session C R513
<b>Registration opens at 11:30 &amp; Lunch</b> (conference desk open every day)	Lunch break 12:00-13:00	Lunch break 12:00-13:00	<b>Poster Awards &amp; Closing</b> 11:40-13:00, R712
<b>Tutorials</b> 12:30-15:30; R711 12:30 Tutorial 1 13:30 Tutorial 2 14:30 Tutorial 3	<b>Board Meeting</b> 12:30-15:00 P603	<b>Plenary Session 2</b> 13:00-15:00 R712	Lunch 13:00
	<b>JEOL workshop</b> 13:30-15:30 Laboratory	<b>Poster Session 1</b> 15:00-17:00 P601,602,604	<b>Poster Session 2</b> 14:20-16:20 P601,602,604
Coffee break 15:30-16:00	Coffee break floor P/L	Coffee break floor P/L	
<b>Opening Awards Ceremony</b> 16:00-19:00 R712	<b>Parallel Sessions 2</b> 17:00 - 18:20 Session A R711 Session B R611 Session C R513	<b>Parallel Sessions 4</b> 16:20 - 17:20 Session A R711 Session B R611 Session C R513	
<b>Welcome Reception</b> 19:00-21:00 K7	<b>Members' Assembly</b> 18:30; R712	<b>Boat Trip</b> Departure 17:30	
	<b>Subgroup-Session EPR</b> following the assembly; R712	<b>Conference Dinner Konzil</b> 19:30 - 22:00	

## Monday, 18 September 2023

Time	Programme	Location/Room
11:30-20:00	Registration (Desk open every day)	Level R5
9:30-12:30	JEOL User Meeting	M630
11:30-12:30	Lunch	Mensa, building K
<b>12:30-15:30</b>	<b>Tutorials</b> <i>Chair: Michael Kovermann</i>	<b>R711</b>
12:30-13:30	<b>Mykhailo Azarkh, University of Konstanz, Germany</b> <i>Product Operator Formalism</i>	
13:30-14:30	<b>Arno P.M. Kentgens, Radboud University Nijmegen, Netherlands</b> <i>Solid-State NMR of Quadrupolar Nuclei</i>	
14:30-15:30	<b>Friedemann Reinhard, University of Rostock, Germany</b> <i>The quest for nanoscale magnetic resonance</i>	
<b>12:30-15:00</b>	<b>Board Meeting</b>	<b>P603</b>
13:30-15:30	JEOL Workshop	NMR-laboratory
15:30-16:00	Coffee break	Foyers R
<b>16:00-19:00</b>	<b>Opening and Awards Ceremony</b> <i>Chair: Malte Drescher</i>	<b>R712</b>
16:00-16:15	<b>Malte Drescher, University of Konstanz, Germany</b> <i>Welcome/Introduction</i>	
16:15-17:45	<b>Ernst awards – Chair: Karsten Seidel</b> - Paolo C. Bruzzese - Ilia Kulikov - Christian F. Pantoja	
17:45-18:15	<b>Albert Overhauser award – Chair: Henrike Heise</b> Leif Antonschmidt	
18:15-19:00	<b>Felix Bloch Lectureship – Chair: Jörg Matysik</b> Loren B. Andreas	
<b>19:00-21:00</b>	<b>Welcome Reception</b>	<b>Mensa, level K7</b>

Tuesday, 19 September 2023

Time	Programme	Location/ Room
<b>8:30-10:30</b>	<b>Plenary Session 1</b> <i>Chair: Arno Kentgens</i>	<b>R712</b>
8:30-9:10	<b>Ilya Kuprov, University of Southampton, United Kingdom</b> <i>Simulation of complex magnetokinetic processes</i>	
9:10-9:50	<b>Ulrich Weininger, Martin-Luther-Universität Halle-Wittenberg, Germany</b> <i>Aromatic Ring Flips in Proteins: Conformational Fluctuations and Their Transition States</i>	
9:50-10:30	<b>Anne Schütz, LMU München, Germany</b> <i>Unravelling ATP processing by a human enzyme at the atomic level</i>	
10:30-11:00	Coffee break	Foyers R
<b>11:00-12:00</b>	<b>Parallel Session 1A - Protein dynamics and relaxation</b> <i>Chair: Katja Petzold</i>	<b>R711</b>
11:00-11:20	<b>Sara Medina-Gomez, TU-Dortmund University, Germany</b> <i>Solid-State NMR Study of the Dynamics of Human p38<math>\alpha</math> MAP Kinase</i>	
11:20-11:40	<b>Albert Smith-Penzel, Universität Leipzig, Germany</b> <i>pyDIFRATE: Deep Insight into Dynamics with NMR and MD</i>	
11:40-12:00	<b>Nils-Alexander Lakomek, Heinrich-Heine-Universität Düsseldorf, Germany</b> <i><sup>15</sup>N NMR relaxation experiments for the investigation of intrinsically disordered proteins at high magnetic fields</i>	
<b>11:00-12:00</b>	<b>Parallel Session 1B - Pulsed dipolar spectroscopy applications</b> <i>Chair: Thomas Prisner</i>	<b>R611</b>
11:00-11:20	<b>Benesh Joseph, Freie Universitaet Berlin, Germany</b> <i>Time-resolved Mn<sup>2+</sup>-NO and NO-NO distance measurements reveal that catalytic asymmetry regulates alternating access in an ABC transporter</i>	
11:20-11:40	<b>Juliane Stehle, University of Konstanz, Germany</b> <i>Hopping of copper(II) ions as event preceding copper-assisted fibrillization of amyloid-beta peptides</i>	
11:40-12:00	<b>Maxim Yulikov, ETH Zurich, Switzerland</b> <i>Describing Structural Ensembles and Local Sites Heterogeneity in Dietary Fibers Solutions by Pulse EPR</i>	
<b>11:00-12:00</b>	<b>Parallel Session 1C – Spectrometer-to-go</b> <i>Chair: Jens Anders</i>	<b>R513</b>
11:00-11:20	<b>Selina Eckel, Karlsruhe Institute of Technology (KIT) , Germany</b> <i>Development of a Broadband On-Chip EPR Spectrometer</i>	
11:20-11:40	<b>Ke Xu, University of Siegen, Germany</b> <i>Fast Sample Spinning by 3D Printing</i>	
11:40-12:00	<b>Rouven Maier, University of Stuttgart, Germany</b> <i>Application of high magnetic fields to micron-scale NMR spectroscopy with quantum sensors in diamond</i>	
12:00-13:00	Lunch break	Mensa

<b>13:00-14:30</b>	<b>Plenary Session 2</b> <i>Chair: Henrike Heise</i>	<b>R712</b>
13:00-13:40	<b>Sabine Richert, University of Freiburg, Germany</b> <i>Exploring spin communication in photogenerated molecular multi-spin systems</i>	
13:40-14:20	<b>Yoh Matsuki, Osaka University, Japan</b> <i>Methods and Instruments for High-Field MAS DNP toward Intracellular Structural Biology</i>	
14:20-15:00	<b>Silvia Cavagnero, University of Wisconsin-Madison, United States</b> <i>Nuclear-Spin Hyperpolarization of Amino Acids and Proteins in Solution via LC-photo-CIDNP</i>	
15:00-17:00	Coffee break parallel to poster session	P/L6
<b>15:00-17:00</b>	<b>Poster Session 1</b>	<b>Level P6</b>
<b>17:00-18:20</b>	<b>Parallel Session 2A - Advanced NMR applications</b> <i>Chair: Michael Kovermann</i>	<b>R711</b>
17:00-17:20	<b>Thomas Wiegand, Max-Planck-Institute for Chemical Energy Conversion, Germany</b> <i>Potentials of solid-state NMR in organic mechanochemistry</i>	
17:20-17:40	Replaced by: <b>Muslim Dvoyashkin, Leipzig University, Germany</b> <i>Capability of In Situ NMR Spectroscopy for Studying Nonequilibrium Nanoconfined Fluids</i>	
17:40-18:00	<b>Sebastian Scheidel, Würzburg University, Germany</b> <i>Life is Short, Make it Sweet: Structure-Property-Relationships of Sugar Surfactant-Boron-Complexes and Their Formulations</i>	
18:00-18:20	<b>Franziska Rüttger, Georg August Universität Göttingen, Germany</b> <i>Boron Signal Assignment in Borane Clusters using <sup>11</sup>B Residual Quadrupolar Couplings</i>	
17:00-18:00	<b>Parallel Session 2B – EPR methods</b> <i>Chair: Mykhailo Azarkh</i>	<b>R611</b>
17:00-17:20	<b>Andreas Meyer, Max-Planck-Institute for Multidisciplinary Sciences, Germany</b> <i>High Resolution <sup>19</sup>F Electron Nuclear Double Resonance for Structural Biology</i>	
17:20-17:40	<b>Joshua Wort, University of Bonn, Germany</b> <i>Enhanced Sensitivity for Pulse Dipolar EPR Spectroscopy Using Variable-time RIDME</i>	
17:40-18:00	<b>Maximilian Gauger, Goethe University Frankfurt, Germany</b> <i>Combining orientation-selective PELDOR and <sup>19</sup>F ENDOR to investigate the conformational dynamics of dsRNA</i>	
<b>17:00-18:20</b>	<b>Parallel Session 2C - Hyperpolarization and spin dynamics</b> <i>Chair: Guinevere Mathies</i>	<b>R513</b>
17:00-17:20	<b>Alex Van der Ham, Max Planck Institut für multidisziplinäre Naturwissenschaften, Germany</b> <i>Hyperpolarization Transfer Experiments for Liquid-state Overhauser Dynamic Nuclear Polarization</i>	
17:20-17:40	<b>Anna Parker, Nvision Imaging Technologies GmbH, Germany</b> <i>Hyperpolarized solution-state NMR spectroscopy via intermolecular NOE utilizing overwhelming source magnetization</i>	
17:40-18:00	<b>Lisa Fries, Max Planck Institut für multidisziplinäre Naturwissenschaften, Germany</b> <i>Real-Time Metabolic Magnetic Resonance Spectroscopic Imaging of Pancreatic and Colon Cancer Tumor-Xenografts with Para-Hydrogen Hyperpolarized 1-<sup>13</sup>C Pyruvate</i>	
18:00-18:20	<b>Marvin Lenjer, Max Planck Institute for Multidisciplinary Sciences, Germany</b> <i>Exploring Spin Dynamics during Electron Spinlock Pulses</i>	
<b>18:30-19:30</b>	<b>Members' Assembly</b>	<b>R712</b>
followed by:	Subgroup-Session EPR	R712

**Wednesday, 20 September 2023**

Time	Programme	Location/ Room
<b>8:30-10:30</b>	<b>Plenary Session 3</b> <i>Chair: Michael Kovermann</i>	<b>R712</b>
8:30-9:10	<b>Roland Riek, ETH Zürich, Switzerland</b> <i>FASTER NMR: On automated protein structure determination and photo-CIDNP based fragment-based drug screening</i>	
9:10-9:50	<b>Jens Anders, University of Stuttgart, Germany</b> <i>MR meets microelectronics: Recent advances in chip-based MR detectors</i>	
9:50-10:30	<b>Katja Petzold, Uppsala University, Sweden</b> <i>RNA dynamics by NMR</i>	
10:30-11:00	Coffee break	Foyers R
<b>11:00-12:00</b>	<b>Parallel Session 3A - Phase separation</b> <i>Chair: Paul Schanda</i>	<b>R711</b>
11:00-11:20	<b>Narsollah Rezaie Ghaleh, Heinrich Heine Universität Düsseldorf, Germany</b> <i>Biomolecular phase separation monitored through combined NMR and EPR probes of dynamics</i>	
11:20-11:40	<b>Jochen Balbach, Martin Luther University Halle-Wittenberg, Germany</b> <i>UV-B damage and liquid-liquid phase separation of eye lens gammaD crystallin</i>	
11:40-12:00	<b>Sanjay Vinod Kumar, Universität Konstanz, Germany</b> <i>Dynamics study by NMR shows inhomogenous structure of amorphous calcium carbonate</i>	
<b>11:00-12:00</b>	<b>Parallel Session 3B - EPR applications</b> <i>Chair: Mykhailo Azarkh</i>	<b>R611</b>
11:00-11:20	<b>Yury Kutin, TU Dortmund University, Germany</b> <i>EPR/ENDOR characterization of triplet vinylidenes</i>	
11:20-11:40	<b>Annalisa Pierro, University of Konstanz, Germany</b> <i>Dealing with the elephant in the room: protein dynamics at the ribosome interface</i>	
11:40-12:00	<b>Bela Bode, University of St Andrews, United Kingdom</b> <i>Investigating protein structure and function through paramagnetic substitution of natively bound metal ions</i>	
<b>11:00-12:00</b>	<b>Parallel Session 3C - Pulse shaping</b> <i>Chair: Ilya Kuprov</i>	<b>R513</b>
11:00-11:20	<b>Martha Wachter-Lehn, Karlsruhe Institute of Technology (KIT), Germany</b> <i>Development of energy-optimized broadband pulses for fast-pulsing 2D NMR experiments</i>	
11:20-11:40	<b>Paul Trenkler, Goethe University Frankfurt am Main, Germany</b> <i>Shaped pulses for broadband excitation and their optimization including the spectrometers transfer function</i>	
11:40-12:00	<b>Hector Cortes Sanchez, Universität Siegen, Germany</b> <i>Echo pulses for background suppression by optimal control</i>	
12:00-13:00	Lunch break	Mensa

<b>13:00-14:20</b>	<b>Plenary Session 4</b> <i>Chair: Karsten Seidel</i>	<b>R712</b>
13:00-13:40	<b>Markus Weingarth, Utrecht University, Netherlands</b> <i>The mechanisms of Lipid-targeting Antibiotics</i>	
13:30-14:20	<b>Tabea Arndt, KIT - Karlsruhe Institute of Technology, Germany</b> <i>Superconducting Magnet Technology – status, trends and prospects</i>	
14:20-16:20	Coffee break parallel to poster session	P/L6
<b>14:20-16:20</b>	<b>Poster Session 2</b>	<b>Level P6</b>
<b>16:20-17:20</b>	<b>Parallel Session 4A - NMR structural biology</b> <i>Chair: Markus Weingarth</i>	<b>R711</b>
16:20-16:40	<b>Franz Hagn, TU Munich – BNMRZ, Germany</b> <i>Structural basis of metabolite transport by the chloroplast outer envelope channel OEP21</i>	
16:40-17:00	<b>Nina Schröder, RWTH Aachen University, Germany</b> <i>ATP-hydrolysis in the P-loop ATPase SufC studied by solid-state NMR</i>	
17:00-17:20	<b>Luis Gardon, Heinrich Heine Universität Düsseldorf, Germany</b> <i>Structural Influence of Pyroglutamylation at Position 3 in an Amyloid <math>\beta</math> (3-42) Fibril Polymorph probed by solid-state NMR</i>	
<b>16:20-17:20</b>	<b>Parallel Session 4B - EPR Discussion</b> <i>Chair: Müge Kasanmascheff</i>	<b>R611</b>
16:20-16:50	<b>Thomas Prisner, Goethe University Frankfurt am Main, Germany</b> <b>Peter Höfer, Bruker BioSpin GmbH, Germany</b> <i>Panel Discussion on EPR</i>	
16:50-17:20	<b>Klaus-Peter Dinse, Germany</b> <i>IES Fellow Award</i>	
<b>16:20-17:20</b>	<b>Parallel Session 4C – Surfaces</b> <i>Chair: Yoh Matsuki</i>	<b>R513</b>
16:20-16:40	<b>Jörn Schmedt auf der Günne, Universität Siegen, Germany</b> <i>NMR at the Surface of Catalytically Active Nano-Scale Materials</i>	
16:40-17:00	<b>Sara Amanzadeh Salout, TU of Dresden, Germany</b> <i>Solid-state NMR investigation of alcohol adsorption by metal–organic frameworks: adsorption state, selectivity, and adsorption-induced phase transitions</i>	
17:00-17:20	<b>Torsten Gutmann, TU Darmstadt, Germany</b> <i>Detection of Nanomolar Amounts of Functional Groups on Paper Substrates by Solid-State Dynamic Nuclear Polarization</i>	
<b>17:30</b>	<b>Departure for Boat Trip</b>	<b>Meeting in foyer R5</b>
<b>19:30-22:00</b>	<b>Conference Dinner</b>	<b>Konzil Building (by Konstanz Train Station)</b>

Thursday, 21 September 2023

Time	Programme	Location/ Room
<b>8:30-10:30</b>	<b>Plenary Session 5</b> <i>Chair: Burkhard Luy</i>	<b>R712</b>
8:30-9:10	<b>Fedor Jelezko, Ulm University, Germany</b> <i>Nanoscale NMR enabled by diamond spin qubits</i>	
9:10-9:50	<b>Warren S. Warren, Duke University, United States</b> <i>Improving SABRE hyperpolarization using non-intuitive fields and sequences</i>	
9:50-10:30	<b>Paul Schanda, Institute of Science and Technology (ISTA), Austria</b> <i>Function-related dynamics in large proteins on multiple length scales from NMR</i>	
10:30-11:00	Coffee break	Foyers R
<b>11:00-11:40</b>	<b>Parallel Session 5A – Antibiotics</b> <i>Chair: Annalisa Pierro</i>	<b>R711</b>
11:00-11:20	<b>Raj Kumar, Utrecht University, Netherlands</b> <i>The mode of action of the lipopeptide antibiotic Daptomycin</i>	
11:20-11:40	<b>Francesca Lavore, Utrecht University, Netherlands</b> <i>NMR studies of the soluble and insoluble ErmB-32merRNA complex in the context of antibiotic resistance</i>	
<b>11:00-11:40</b>	<b>Parallel Session 5B - Diffusion and Imaging</b> <i>Chair: Silvia Cavagnero</i>	<b>R611</b>
11:00-11:20	<b>Robin Allert, Technical University of Munich, Germany</b> <i>Imaging local diffusion in microstructures using NV-based pulsed field gradient NMR</i>	
11:20-11:40	<b>Dilara Faderl, Karlsruhe Institute of Technology, Germany</b> <i>Simultaneous Molecular Imaging of Protein-Ligand Interactions Gives Insights into Drug Discovery</i>	
<b>11:00-11:40</b>	<b>Parallel Session 5C - 2D COFs</b> <i>Chair: Fedor Jelezko</i>	<b>R513</b>
11:00-11:20	<b>Nikolaj Lopatik, TU Dresden, Germany</b> <i>Solid-state NMR Investigations of 2D Materials</i>	
11:20-11:40	<b>Arafat Khan, Technische Universität Dresden, Germany</b> <i>Ex situ and operando NMR studies of redox two-dimensional covalent organic framework (2D-COFs) cathodes for durable aluminum batteries</i>	
<b>11:40-13:00</b>	<b>Awards and Closing</b> <i>Chair: Jörg Matysik</i>	<b>R712</b>
11:40-12:10	<b>Otto-Stern award</b>	
12:10-12:40	<b>Honorary membership</b> <b>Harald Günther</b>	
12:40-13:00	<b>Poster awards and Closing</b>	
13:00	Lunch	Mensa



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