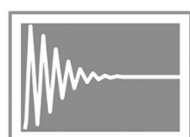


44th FGMR Annual Discussion Meeting 2023

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
	Plenary Session 1 08:30 - 10:30 R712	Plenary Session 3 08:30 - 10:30 R712	Plenary Session 5 08:30 - 10:30 R712
	Coffee break 10:30-11:00	Coffee break 10:30-11:00	Coffee break 10:30-11:00
JEOL user meeting 9:30-12:30 M630	Parallel Sessions 1 11:00 - 12:00 Session A R711 Session B R611 Session C R513	Parallel Sessions 3 11:00 - 12:00 Session A R711 Session B R611 Session C R513	Parallel Sessions 5 11:00 - 11:40 Session A R711 Session B R611 Session C R513
Registration opens at 11:30 & Lunch (conference desk open every day)	Lunch break 12:00-13:00	Lunch break 12:00-13:00	Poster Awards & Closing 11:40-13:00, R712
Tutorials 12:30-15:30; R711 12:30 Tutorial 1 13:30 Tutorial 2 14:30 Tutorial 3	Board Meeting 12:30-15:00 P603	Plenary Session 2 13:00-15:00 R712	Lunch break 13:00-13:30
	JEOL workshop 13:30-15:30 Laboratory	Poster Session 1 15:00-17:00 P601,602,604	Subgroup-Sessions 13:30-15:30 Subgroup 1 R711 Subgroup 2 R611 Subgroup 3 R513
Coffee break 15:30-16:00		Coffee break floor P/L	
Opening Awards Ceremony 16:00-19:00 R712	Parallel Sessions 2 17:00 - 18:20 Session A R711 Session B R611 Session C R513	Poster Session 2 14:20-16:20 P601,602,604	
Welcome Reception 19:00 K7	Members' Assembly 18:30 R712	Parallel Sessions 4 16:20 - 17:20 Session A R711 Session B R611 Session C R513	
		Boat Trip Departure 17:30	
		Conference Dinner Konzil 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
12:30-15:00	Tutorials <i>Chair: Michael Kovermann</i>	R711
12:30-15:00	Mykhailo Azarkh, University of Konstanz <i>Product Operator Formalism</i>	
12:30-15:00	Arno P.M. Kentgens, Radboud University Nijmegen <i>Solid-State NMR of Quadrupolar Nuclei</i>	
12:30-15:00	Friedemann Reinhard, University of Rostock <i>The quest for nanoscale magnetic resonance</i>	
12:30-15:00	Board Meeting	P603
13:30-15:30	JEOL Workshop	NMR-laboratory
15:30-16:00	Coffee break	Foyers R
16:00-19:00	Opening and Awards Ceremony <i>Chair: Malte Drescher</i>	R712
16:00-16:15	Malte Drescher, University of Konstanz <i>Welcome/Introduction</i>	
16:15-17:45	Ernst awards – Chair: Karsten Seidel	
17:45-18:15	Albert Overhauser award – Chair: Henrike Heise	
18:15-19:00	Felix Bloch Lectureship – Chair: Jörg Matysik	
19:00	Welcome Reception	Mensa, level K7

Tuesday, 19 September 2023

Time	Programme	Location/ Room
8:30-10:30	Plenary Session 1 <i>Chair: Arno Kentgens</i>	R712
8:30-9:10	Ilya Kuprov, University of Southampton <i>Simulation of complex magnetokinetic processes</i>	
9:10-9:50	Ulrich Weininger, Martin-Luther-Universität Halle-Wittenberg <i>Aromatic Ring Flips in Proteins: Conformational Fluctuations and Their Transition States</i>	
9:50-10:30	Anne Schütz, LMU München <i>Unravelling ATP processing by a human enzyme at the atomic level</i>	
10:30-11:00	Coffee break	Foyers R
11:00-12:00	Parallel Session 1A - Protein dynamics and relaxation <i>Chair: Katja Petzold</i>	R711
11:00-11:20	Sara Medina-Gomez, TU-Dortmund University <i>Solid-State NMR Study of the Dynamics of Human p38α MAP Kinase</i>	
11:20-11:40	Albert Smith-Penzel, Universität Leipzig <i>pyDIFRATE: Deep Insight into Dynamics with NMR and MD</i>	
11:40-12:00	Nils-Alexander Lakomek, Heinrich-Heine-Universität Düsseldorf <i>¹⁵N NMR relaxation experiments for the investigation of intrinsically disordered proteins at high magnetic fields</i>	
11:00-12:00	Parallel Session 1B - Pulsed dipolar spectroscopy applications <i>Chair: Thomas Prisner</i>	R611
11:00-11:20	Benesh Joseph, Freie Universität Berlin <i>Time-resolved Mn²⁺-NO and NO-NO distance measurements reveal that catalytic asymmetry regulates alternating access in an ABC transporter</i>	
11:20-11:40	Juliane Stehle, University of Konstanz <i>Hopping of copper(II) ions as event preceding copper-assisted fibrillization of amyloid-beta peptides</i>	
11:40-12:00	Maxim Yulikov, ETH Zurich <i>Describing Structural Ensembles and Local Sites Heterogeneity in Dietary Fibers Solutions by Pulse EPR</i>	
11:00-12:00	Parallel Session 1C – Spectrometer-to-go <i>Chair: Jens Anders</i>	R513
11:00-11:20	Selina Eckel, Karlsruhe Institute of Technology (KIT) <i>Development of a Broadband On-Chip EPR Spectrometer</i>	
11:20-11:40	Ke Xu, University of Siegen <i>Fast Sample Spinning by 3D Printing</i>	
11:40-12:00	Rouven Maier, University of Stuttgart <i>Application of high magnetic fields to micron-scale NMR spectroscopy with quantum sensors in diamond</i>	
12:00-13:00	Lunch break	Mensa

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

Wednesday, 20 September 2023

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

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

Thursday, 21 September 2023

Time	Programme	Location/ Room
8:30-10:30	Plenary Session 5 <i>Chair: Burkhard Luy</i>	R712
8:30-9:10	Fedor Jelezko, Ulm University <i>Nanoscale NMR enabled by diamond spin qubits</i>	
9:10-9:50	Warren S. Warren, Duke University <i>Improving SABRE hyperpolarization using non-intuitive fields and sequences</i>	
9:50-10:30	Paul Schanda, Institute of Science and Technology Austria (ISTA) <i>Function-related dynamics in large proteins on multiple length scales from NMR</i>	
10:30-11:00	Coffee break	Foyers R
11:00-11:40	Parallel Session 5A – Antibiotics <i>Chair: Annalisa Pierro</i>	R711
11:00-11:20	Raj Kumar, Utrecht University, Netherlands <i>The mode of action of the lipopeptide antibiotic Daptomycin</i>	
11:20-11:40	Francesca Lavore, Utrecht University <i>NMR studies of the soluble and insoluble ErmB-32merRNA complex in the context of antibiotic resistance</i>	
11:00-11:40	Parallel Session 5B - Diffusion and Imaging <i>Chair: Silvia Cavagnero</i>	R611
11:00-11:20	Robin Allert, Technical University of Munich <i>Imaging local diffusion in microstructures using NV-based pulsed field gradient NMR</i>	
11:20-11:40	Dilara Faderl, Karlsruhe Institute of Technology <i>Simultaneous Molecular Imaging of Protein-Ligand Interactions Gives Insights into Drug Discovery</i>	
11:00-11:40	Parallel Session 5C - 2D COFs <i>Chair: Fedor Jelezko</i>	R513
11:00-11:20	Nikolaj Lopatik, TU Dresden <i>Solid-state NMR Investigations of 2D Materials</i>	
11:20-11:40	Arafat Khan, Technische Universität Dresden <i>Ex situ and operando NMR studies of redox two-dimensional covalent organic framework (2D-COFs) cathodes for durable aluminum batteries</i>	
11:40-13:00	Awards and Closing <i>Chair: Jörg Matysik</i>	R712
11:40-12:10	Otto Stern award	
12:10-12:40	Honorary Membership	
12:40-13:00	Poster awards and Closing	
13:00-13:30	Lunch break	Mensa
13:30-15:30	Subgroup Sessions	R711, R611, R513

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