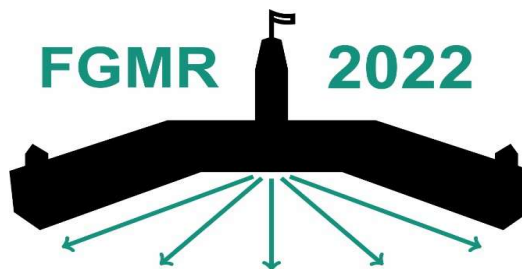


# Program



**Venue: Audimax and EBI Hörsaal, Karlsruhe Institute of Technology**

<b>Monday 12 September</b>	<b>12.00 - 19.00</b>	<b>Registration</b>	<b>Audimax Foyer</b>
	<b>13.15 - 15.30</b>	<b>Tutorials</b>	<b>Audimax I</b>
	13.15	<i>Steffen Glaser</i>	
	14.00	Dynamics in Magnetic Resonance: Approaches to Characterizing the Fourth Dimension <i>Albert Smith-Penzel, Germany</i>	
	14.45	Polarization transfer in solids <i>Guinevere Mathies, Germany</i>	
	<b>15.30 - 16.10</b>	<b>Coffee Break</b>	<b>Audimax Foyer</b>
	<b>16.10 - 16.20</b>	<b>Opening</b>	<b>Audimax Foyer</b>
	<b>16.20 - 19.00</b>	<b>Awards</b>	<b>Audimax I</b>
	16.20	Ernst-Awards	
	17.40	Felix Bloch Lecture: <i>Dominik Bucher, Germany</i> Diamond quantum sensors for nano- and microscale NMR spectroscopy	
	18.15	Otto Stern Award: <i>Jörg Kärger, Germany</i> The Rich Harvest of Diffusion NMR with Guest Molecules in Nanoporous Materials	
	<b>19.00 - 21.00</b>	<b>Welcome Mixer</b>	

Tuesday 13 September

Program



08.00 - 19.00	Registration	Audimax Foyer
08.30 - 10.15	Plenary Session 1   Chair: TBA	Audimax I
08.30	Plenary Speaker 1: <i>Lucio Frydman, Israel</i> Polarization and depolarization routes to enhance the sensitivity of solution and solid state NMR	
09.05	Plenary Speaker 2: <i>Eric McInnes, UK</i> Heavy metal EPR spectroscopy	
09.40	Plenary Speaker 3: <i>Katalin E. Kövér, Hungary</i> Combined NMR Experiments for Rapid Resonance Assignment of Small-to-Medium Size Molecules	
10.15 - 10.45	Coffee Break	Audimax Foyer
10.45 - 12.15	Parallel Sessions	
10.45	<b>Parallel Session 1: Computation   Chair: TBA</b> Structure and dynamics of proteins and domains involved in synaptic transmission <i>Zoltán Gáspári, Hungary</i>	<b>Audimax I</b>
11.10	Automated biomolecular NMR spectra analysis, assignments, and structures with the deep learning technique ARTINA <i>Peter Güntert, Germany</i>	
11.35	Understanding Contact Shifts in Paramagnetic Coordination Compounds <i>Scott Kraeker, Canada</i>	
11.55	Flow encoding established by optimal control RF pulse <i>Mehrdad Alinaghian Jouzdani, Germany</i>	
10.45	<b>Parallel Session 2: Exotica   Chair: TBA</b> Studies of short-lived nuclei and their interactions through the lens of beta-NMR <i>Beatrice Karg, Switzerland</i>	<b>Audimax II</b>
11.10	Nanoscale magnetic resonance enabled by diamond spin qubits <i>Fedor Jelezko, Germany</i>	
11.35	Transition Metal NMR as a Guide for Catalyst Development <i>Markus Leutzsch, Germany</i>	
11.55	EDNMR spectroscopy to detect water binding to nitroxide radicals <i>Lisa Fries</i>	
10.45	<b>Parallel Session 3: Energy &amp; Materials   Chair: TBA</b> NMR/MRI analysis of failure mechanisms of Li metal batteries <i>Günther Brunklaus, Germany</i>	<b>EBI-Hörsaal</b>
11.10	Accurate Determination of Exchange Interactions in Biomimetic Peroxidocopper(II) Complexes <i>Alexander Schnegg, Germany</i>	
11.35	EPR spectroscopic investigation of Lithium-organic batteries <i>Davis T. Daniel, Germany</i>	
11.55	NMR Investigations on Electrode and Electrolyte Materials for Li-Ion Batteries <i>Sylvia Indris, Germany</i>	
12.15 - 13.30	Lunch	Audimax Foyer
	Magritek Symposium	Audimax I
13.30 - 15.00	Parallel Sessions	
13.30	<b>Parallel Session 4: Structure   Chair: TBA</b> Stereochemical Elucidation of Marine Natural Products using Residual Chemical Shift Anisotropy from a Liquid Crystalline Phase <i>Han Sun, Germany</i>	<b>Audimax I</b>
13.55	Dynamic organization of a chaperone network in the human endoplasmic reticulum <i>Sebastian Hiller, Switzerland</i>	
14.20	Directed evolution of conformational dynamics in an epigenetic reader protein <i>Rasmus Linser, Germany</i>	
14.40	Validating structure predictions with nanomolar sensitivity – a new era for pulse dipolar EPR spectroscopy <i>Bela Bode, UK</i>	
13.30	<b>Parallel Session 5: Diffusion &amp; Imaging   Chair: G. Guthausen</b> Advanced NMR cryoporometry characterization of mesoporous solids <i>Rustum Valiullin, Germany</i>	<b>Audimax II</b>
13.55	Fully biocompatible h- <sup>1</sup> H- <sup>13</sup> C pyruvate for metabolic investigations <i>Francesca Reineri, Italy</i>	
14.20	In vivo imaging of extracellular pH using hyperpolarized <sup>13</sup> C-labelled biosensors <i>Franz Schilling, Germany</i>	
14.40	Highly fluorinated peptides as probes for in vivo <sup>19</sup> F-MRI <i>Stephan L. Grage, Germany</i>	
13.30	<b>Parallel Session 6: Dynamic Nuclear Polarization   Chair: B. Meier</b> Biomolecular phase transitions by non-equilibrium NMR <i>Dennis Kurbach, Austria</i>	<b>EBI-Hörsaal</b>
13.55	Photo-Induced Reactivity followed by EPR and NMR <i>Georg Gescheidt-Demner, Austria</i>	
14.20	Protein-RNA long-range contacts by cross relaxation and rotational resonance under MAS-DNP <i>Bernd Corzilius, Germany</i>	
14.40	Hyperpolarized Solution-State NMR Spectroscopy via intermolecular NOE <i>Ilai Schwartz, Germany</i>	
15.00 - 17.00	Poster Session 1 and Coffee Break	Audimax Foyer
17.00 - 18.30	Parallel Sessions	
17.00	<b>Parallel Session 7: Liquids   Chair: TBA</b> Intrinsically Disordered Proteins: Global and Atomic Level Characterization <i>Andrea Bodor, Hungary</i>	<b>Audimax I</b>
17.25	Mapping structural epitopes on small proteins interacting with intact mAbs using hydrogen/deuterium exchange memory NMR <i>Mario Schubert, Austria</i>	
17.50	Structural dynamics of intrinsically disordered proteins at the membrane interface: New NMR insights into the pre-fusion state of SNARE proteins <i>Nils A. Lakomek, Germany</i>	
18.10	Connection of Isolated Stereoclusters by Combining <sup>13</sup> C-RCSA, RDC and Structural Revision of a Tetraprenyltoluquinol Chromane Meroterpenoid from <i>Sargassum muticum</i> <i>Juan C. Fuentes-Monteverde, Germany</i>	
17.00	<b>Parallel Session 8: Quantum Information Technology   Chair: TBA</b> Tuning spin communication in photogenerated three-spin systems for molecular spintronics <i>Sabine Richert, Germany</i>	<b>Audimax II</b>
17.25	Enhanced sensitivity ESR and spin-based quantum memories <i>John J. L. Morton, UK</i>	
17.50	Molecular Qubits: Switching, Self-Assembly and Strong Coupling <i>Joris van Slageren, Germany</i>	
18.10	tba	
17.00	<b>Parallel Session 9: Low-Field NMR   Chair: TBA</b> Integrated and Networked Systems and Processes - How NMR Spectroscopy Can Transform our Chemical and Pharmaceutical Production <i>Michael Maiwald, Germany</i>	<b>EBI-Hörsaal</b>
17.25	Paramagnetic <sup>7</sup> Li MAS NMR in a Permanent Magnet <i>Jörn Schmiedt auf der Günne, Germany</i>	
17.50	Composition Analysis of Complex Gaseous Mixtures by High-Pressure <sup>1</sup> H Low-Field NMR Spectroscopy and Indirect Hard Modeling <i>Sergio A. Ortiz Restrepo, Germany</i>	
18.10	Benchmark 80 <sup>1</sup> H MHz NMR spectrometer as online HPLC detector <i>Markus Matz, Germany</i>	
18.30	FGMR Member's Meeting	EBI-Hörsaal
19.00	Guided City Tours	
19.30	AK EPR	EBI-Hörsaal
19.30	AK Small Molecules	TBA

Wednesday 14 September

Program



08.00 - 19.00	Registration	Audimax Foyer
08.30 - 10.15	Plenary Session 2   Chair: TBA	Audimax I
08.30	Plenary Speaker 4: <i>Ruth M. Gschwind, Germany</i> NMR in Organo- and Photocatalysis – Pushing the Limits	
09.05	Plenary Speaker 5: <i>Malcom H. Levitt, UK</i> Path-Sum: a new Avenue for Spin Dynamics	
09.40	Plenary Speaker 6: <i>Maxie Rössler, UK</i> Controlling and exploiting intrinsic unpaired electrons in metalloproteins	
10.15 - 10.45	Coffee Break	Audimax Foyer
10.45 - 12.15	Parallel Sessions	
10.45	Parallel Session 10: Beyond Boltzmann   Chair: TBA Adventures with para-hydrogen in biochemistry and biology <i>Stefan Gläggler, Germany</i>	Audimax I
11.10	An integrative cryo-EM and EPR approach to unveil the steps of a prepore-to-pore transition of a Tc toxin <i>Enrica Bordignon, Switzerland</i>	Parallell Session 11: Biological Systems   Chair: TBA Exploring the Dynamic World of Membrane Systems and Biocatalysis <i>Manuel Etzkorn, Germany</i>
11.35	Low-field Relaxation via Radical Non-Zeeman Reservoir in Solid Pyruvic Acid <i>Michael Jurkatat, Germany</i>	Parallell Session 12: Sustainability & Catalysis   Chair: TBA In situ EPR: A Unique Tool to Monitor Electron Transfer in Working Catalysts <i>Angelika Brückner, Germany</i>
11.55	Hydrogen catalysis of the [Fe]-hydrogenase studied by parahydrogen enhanced NMR <i>Lukas Kaltschnee, Germany</i>	Parallell Session 12: Sustainability & Catalysis   Chair: TBA Metalloradical Catalysis via 'Carbene Radicals' <i>Bas de Bruin, The Netherlands</i>
12.15 - 13.30	Lunch	Audimax Foyer
12.20	Bruker Symposium	Audimax I
13.30 - 15.00	Parallel Sessions	
13.30	Parallel Session 13: In Cell & In Situ   Chair: TBA Discovery of an unknown radical signal in the oxygen-resistant [FeFe]-hydrogenase <i>Müge Kasanmascheff, Germany</i>	Audimax I
13.55	Microfluidic Magnetic Resonance And Hyperpolarisation: New Tools To Study Biological Systems <i>Marcel Utz, UK</i>	Parallel Session 14: Legal Matters & Quality Control   Chair: T. Kuballa Application of NMR spectroscopy in food control <i>Carsten Faulstich, Germany</i>
14.20	In situ and ex situ NMR studies to understand the role of MOF in moderating Pt-Vulcan catalyst for alcohol electrooxidation <i>Arafat H. Khan, Germany</i>	Parallel Session 14: Legal Matters & Quality Control   Chair: T. Kuballa The Use of NMR and qNMR for the Characterisation of European Pharmacopoeia Reference Standards <i>Matthias Weber, France</i>
14.40	Multinuclear Flow MAS NMR for Studying CO <sub>2</sub> -based Sorption-, Capture- and Hydrogenation Processes over the Nanoporous Solids <i>Muslim Dvoyashkin, Germany</i>	Parallel Session 15: Spin Dynamics   Chair: TBA Exploiting the Aharonov-Anandan phase for double-quantum excitation in strongly coupled spin-pairs <i>Christian Bengs, UK</i>
15.00 - 17.00	Poster Session 2 and Coffee Break	Audimax Foyer
17.00 - 18.10	Plenary Session 3   Chair: TBA	Audimax I
17.00	Plenary Speaker 7: <i>Alexander B. Barnes, Switzerland</i> Enabling In-Cell NMR with Pulsed DNP, Electron Decoupling, MAS Spheres and Compact 30 Tesla Magnets	
17.35	Plenary Speaker 8: <i>Anke Henning, US</i> Metabolic MRI at ultra-high fields – from systems architecture to application	
18.10	Free Time / Departure for Conference Dinner	
19.00 - 00.00	Conference Dinner	Palazzo Halle

Thursday 15 September

Program



08.00 - 13.00	Registration	Audimax Foyer
<b>08.30 - 10.00 Parallel Sessions</b>		
08.30	<b>Parallel Session 16: Solids   Chair: TBA</b> Effective Hamiltonian Based Pulse-Sequence Optimization <i>Matthias Ernst, Switzerland</i>	<b>Audimax I Paralell Session 17: Hardware &amp; Miniaturization   Chair: J. Korvink</b> Ultra-high field Magnetic Resonance Imaging and Localized Spectroscopy: Opportunities and challenges for biological specimens <i>Julia Krug, The Netherlands</i>
08.55	<b>Intrinsic paramagnetic susceptibility tensors and applications to GPCRs and high-energy states of proteins</b> <i>Daniel Häussinger, Switzerland</i>	<b>Probing Spin Dynamics using EPR-on-a-Chip</b> <i>Michal Kern, Germany</i>
09.20	<b>Molecular guiding principles behind liquid droplet maturation unravelled by solid-state NMR spectroscopy</b> <i>Thomas Wiegand, Germany</i>	<b>H-MAS update</b> <i>Ago Samoson, Estonia</i>
09.40	<b>Proton-decoupled 15N R1ρ experiment in solid proteins</b> <i>Alexey Krushelnitsky, Germany</i>	<b>Development of a 3D printed ceramic reactor and a custom-made probe head for spatially-resolved operando NMR experiments of flow-through systems</b> <i>Andrea C. Hurtado Rivera, Germany</i>
		<b>Audimax II Paralell Session 18: Food &amp; Health   Chair: T. Kuballa</b> Classification Models and Metabolite Identification: The two Sides of the same Coin <i>Thomas Hackl, Germany</i>
		<b>The Deuteron NMR Hahn Echo Decay in Polyethylene oxide melts</b> <i>Kevin Lindt, Germany</i>
		<b>Structural Investigation of Cu-ZIF-8 by CW and Pulsed Electron Paramagnetic Resonance Techniques</b> <i>Muhammad F. Lukman, Germany</i>
		<b>Hydrogen bonds, charge compensation and packing in polyelectrolyte complexes</b> <i>Ulrich Scheler, Germany</i>
10.00 - 10.30	Coffee Break	Audimax Foyer
<b>10.30 - 12.15 Plenary Session 4   Chair: TBA</b>		
10.30	<b>Plenary Speaker 9: Martin Tollinger, Austria</b> NMR spectroscopic tools to explore the many facets of food allergy	<b>Audimax I</b>
11.05	<b>Plenary Speaker 10: Christian Bonhomme, France</b> Path-Sum: a new Avenue for Spin Dynamics	
11.10	<b>Plenary Speaker 11: Thomas Prisner, Germany</b> Spin Counting by pulsed EPR Methods	
12.15 - 12.55	Honorary Membership Stefan Berger & Wolfgang Lubitz	<b>Audimax I</b>
12.55	Closing	