

Program Schedule

DNP Satellite Meeting

Monday, Sept 29, 2014, BBAW, Markgrafenstr. 38, 10117 Berlin

09:00	Welcome by Shimon Vega (Rehovot)	
	DIP - DNP Session 1 <i>Chair: Shimon Vega</i>	Leibniz-Saal
09:10	Marina Bennati (Göttingen) Recent Insights in Overhauser DNP in Liquids at 0.3 and 3 Tesla	
09:40	Umit Akbey (Berlin) DNP of Proteins and Silicates: New Radicals and Higher Temperatures	
10:00	Vasyl Denysenkov (Frankfurt/M) Overhauser DNP Experiments on Oriented Lipid Bilayers at 9.4 T: Setup and Applications	
10:20	Or Szekely (Rehovot) Sensitizing Protein NMR by Nuclear Hyperpolarization Methods	
10:40	<i>Coffee Break</i>	
11:10	Jan-Henrik Ardenkjaer-Larsen (Lyngby) Hyperpolarized Metabolic Imaging: Preclinical and Clinical Progress	
11:40	Akiva Feintuch (Rehovot) Static and MAS DNP. Similarities and Differences	
12:00	Daphna Shimon (Rehovot) Hetero-Nuclear Polarization Exchange During DNP	
12:20	Discussion time	
12:40	<i>Lunch</i>	
	DIP - DNP Session 2 <i>Chair: Hartmut Oschkinat</i>	Leibniz-Saal
13:30	Geoffrey Bodenhausen (Lausanne) Technical Improvements for Dissolution DNP	
14:00	Andriy Marko (Frankfurt/M) Role of Dipolar Electron Spin-Spin Interaction in High Field DNP Experiments in Liquid Solutions	
14:20	Christian Bretschneider (Rehovot) DNP in Diamond	
14:40	Discussion time	
15:00	Internal Discussion of DIP Project Members <i>Chair: Shimon Vega and Hartmut Oschkinat</i>	

FGMR2014

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15:00	Registration BBAW Markgrafenstr. 38 Foyer	Educational Session <i>Chair:</i>	Leibniz-Saal
16:30		Gunnar Jeschke (Zürich) Advanced EPR for NMR spectroscopists	
17:30		Shimon Vega (Rehovot) Advanced DNP for Beginners	
18:30	<i>Welcome Mixer & Snacks</i>		
19:00	Welcome / Opening remarks		
19:10	Presentation of the FGMR-Award <i>Chair: Christina Thiele and Marina Bennati</i>		Leibniz-Saal
19:30	FGMR Honory Member Robert G. Griffin (Cambridge, USA) Overhauser Effects in Insulating Solids		
20:15	Presentation of the Ernst-Awards <i>Chair: Wolfgang Jahnke</i>		Leibniz-Saal
20:25	Moritz Schmidt (Konstanz) A Genetically Encoded Spin Label for Electron Paramagnetic Resonance Distance Measurements		

20:45	Nanette Jarenwattananon (Los Angeles) Thermal Maps of Gases in Heterogeneous Reactions
21:05	David Schulze-Suenninghausen (Karlsruhe) Rapid Heteronuclear Single Quantum Correlation NMR Spectra at Natural Abundance

Tuesday, Sept 30, 2014, Campus Buch, MDC.C, Robert-Rössle-Str. 10, 13125 Berlin

Plenary I: Frontiers in Magnetic Resonance		Axon I
<i>Chair: Jochen Balbach</i>		
09:00	Lucio Frydman (Rehovot) Emerging Opportunities in High-Sensitivity ¹ H and ¹³ C <i>In Vivo</i> Magnetic Resonance	
09:30	Thomas Prisner (Frankfurt a. M.) New Methodical Aspects for Dipolar Spectroscopy	
10:00	Christian Hilty (College Station) Dissolution DNP in Chemistry	
10:30	<i>Coffee Break</i>	
Plenary II: Imaging		Axon I
<i>Chair: Bernhard Blümich</i>		
11:00	Peter Jezzard (Oxford) New MRI Methods for Assessment of Cerebrovascular Disease	
11:30	Jens Frahm (Göttingen) Magnetic Resonance Imaging in Real Time	
12:00	Klaas Prüssmann (Zürich) Advances in NMR Magnetometry for MRI Applications	
12:30	<i>Lunch</i>	
A1: Materials & Small Molecules		Axon II
<i>Chair: Christina Thiele</i>		
13:30	Ernst Rössler (Bayreuth) Field-Cycling NMR Relaxometry Investigating Soft Matter	
13:55	Eike Brunner (Dresden) Solid-state NMR and SENS DNP Studies of Diatom Biosilica	
14:20	Benno Meier (Southampton) Electric Detection of Ortho and Para Water in Fullerene Cages	
14:35	Hideto Matsuoka (Bonn) Time-Resolved EPR and DFT Studies of Organic Electroluminescent Materials	
14:50	Ulrich Scheler (Dresden) Interfaces and Dynamics in Polymer Composite Materials	
15:05	Daniel Gunzelmann (Geelong) Decoupled Na ⁺ ion Conduction in Poly-AMPS Based Ionomer Electrolytes by Solid-State NMR	
B1: BioMR-Applications		Axon I
<i>Chair: Enrica Bordignon</i>		
	Jochen Balbach (Halle) <i>Ex vivo</i> NMR during PTH Hormone Phosphorylation and Alzheimer Amyloid Formation	
	Christiane Ritter (Stöckheim) Solid-state NMR Structure of the Helical Signal Transduction Filament MAVS	
	Aaron Hahn (Berlin) Site-Directed Spin Labelling of Sulfite Oxidase Using Non-Natural Amino Acids	
	Franziska Kappert (Frankfurt) Structural Characterization of FGFR-Ligand Interaction by NMR Spectroscopy	
	Johann Klare (Osnabrück) Conformational Heterogeneity of Roc Domains in WT and Mutant <i>C. tepidum</i> Roc-COR	
	Manuel Etzkorn (Düsseldorf) Non-Conventional Approaches for the NMR Characterization of Membrane Proteins	
15:20	<i>Coffee Break</i>	
A2: Signal Enhancement Techniques		Axon II
<i>Chair: Marina Bennati</i>		
15:50	Anne Lesage (Lyon) Determining the Conformation of Surface Species by DNP Enhanced Solid-State NMR	
16:15	Shimon Vega (Rehovot) Indirect Double Cross Effect DNP on Heteronuclear Spin Systems	
16:40	Björn Corzilius (Frankfurt a. M.) ¹ H, ¹³ C, and ¹⁵ N Direct Solid Effect DNP with Gd(III)	
16:55	Stefan Glöggler (UCLA) Hyperpolarisation of Unprotected Amino Acid Derivates Utilizing	
B2: NMR in Chem. Biology and Drug Design		Axon I
<i>Chair: Wolfgang Jahnke</i>		
	Gregg Siegal (Leiden) NMR as a Structural Biology Tool for Drug Discovery – Making a Comeback	
	Geoffrey Bodenhausen (Paris) Study of Ligand-Protein Interactions by Combining DNP with Long-Lived States	
	Brigitte Fiege (Basel) A Combination of NMR and X-Ray Crystallography Reveals the Fine Details of Mannoside Binding to FimH Lectin	
	Heiko M. Möller (Potsdam) NMR Studies with the 216 kDa Transmembrane Enzyme	

	PHIP in Water	Complex Na ⁺ -NQR from <i>V. cholerae</i>
17:10	Chris Witte (Berlin) MRI of Hyper-CEST Xenon Biosensors Targeted to Cell-Surface Glycans	Sonja Dames (Garching) Phosphorylation Induced Dynamic Changes Facilitate Estrogen Independent Coactivator Binding to ER β
17:25	Roberto Rizzato (Göttingen) Sensitivity Enhancement in ENDOR by Cross Polarisation and Relaxation	Veronika Kropf (Regensburg) Modulation of the Conformational Equilibrium of Activated Ras by Potential Drug Compounds
18:00	Poster Session 1 (odd numbers presenting)	
18:30	<i>Wine and Cheese – Informal Snacks and Drinks, Poster Session continued</i>	
20:00	FGMR member meeting	

Wednesday, Oct 1, 2014, Campus Buch, MDC.C, Robert-Rössle-Str. 10, 13125 Berlin

	Plenary III: Small Molecules & Materials <i>Chair: Kay Saalwächter</i>		Axon I
09:00	Lyndon Emsley (Lyon) DNP Enhanced Solid-State NMR Spectroscopy		
09:30	Christina Thiele (Darmstadt) Recent Advances in Orienting Organic Compounds for RDC Structural Analysis		
10:00	Gerd Buntkowsky (Darmstadt) Applications of Solid State NMR in Heterogeneous Catalysis		
10:30	<i>Coffee Break</i>		
	A3: Dynamics and Computational Methods <i>Chair: Steffen Glaser</i>	B3: BioMR applications <i>Chair: Leif Schröder</i>	Axon II / Axon I
11:00	Kay Saalwächter (Halle) Rotational and Translational Diffusion in Crowded Protein Solutions	Philipp Selenko (Berlin) Cells, Drugs and NMR	
11:25	Thomas Heydenreich (Garching) Obtaining Insight into Spin Manipulation: Time-Frequency Representation of NMR Pulses	A. Alia (Leiden) <i>In Vivo</i> ¹ H MRI and Localized Spectroscopic Analysis of Alzheimer's Disease in Mouse Models	
11:50	Johannes Weber (Siegen) Linking ³¹ P Magnetic Shielding Tensors to Crystal Structures	Steffen Goerke (Heidelberg) The Signature of Protein Unfolding in CEST Imaging	
12:05	Janosch Hennig (Neuherberg) Combining NMR and Small-Angle Neutron Scattering to Study Protein-RNA Complexes	Daniela Lalli (Florenz) Studying the Ferritin Nanocage by NMR	
12:20	<i>Lunch</i>		
	A4: BioMR – Methods & Apps <i>Chair: Eike Brunner</i>	B4: Materials & Small Molecules <i>Chair: Johannes Liermann</i>	Axon I / Axon II
13:15	Daniella Goldfarb (Rehovot) Probing Protein Conformation in Cells by EPR Distance Measurements Using Gd ³⁺ Spin Labeling	Jürgen Senker (Bayreuth) Studying the Nucleation of Supramolecular Polymer Additives with NMR Crystallography	
13:40	Bernd Reif (Garching) Amyloid Aggregates and Large Soluble Protein Complexes	Claudia Schmidt (Paderborn) Effects of Micellization and Aggregate Growth on the NMR Spectra of Surfactants	
14:05	Jörg Matysik (Leipzig) The Solid-State Photo-CIDNP Effect	Bernhard Blümich (Aachen) Compact NMR: Non-Destructive Testing and Real-Time Spectroscopy	
14:30	Müge Kasanmascheff (Freiburg) Insights into the FeMo Cofactor of Nitrogenase	Maryia Sin (Dresden) Quantitative ¹ H Spectroscopy in Studies of Liquid-Phase Adsorption on Porous Materials	
14:45	Garima Jaipuria (Göttingen) The 18 kDa Translocator Protein in a Lipid Bilayer	Philipp Selter (Münster) Synthesis and Characterization of PAS-PPO Co-Polymers for Li ⁺ Batteries	

15:00	Wiktor Kozminski (Warschau) New High Dimensionality Experiments for Intrinsically Disordered Proteins	Alicia Lund (Santa Barbara) Directly Probing Surface ^{27}Al in Al-SBA-15 with Static and MAS DNP
15:15	Rasmus Linser (Göttingen) Ultra-Sparse-NUS, Diagonal-Compensated 4D Spectroscopy for Facilitated Structure Determination	Dmitry Akhmetzyanov (Frankfurt a. M.) PELDOR on High Spin Mn^{2+} Coupled with a Nitroxide Radical
15:30	<i>Coffee Break</i>	
	Plenary IV: Public Lectures <i>Chair: Hartmut Oschkinat</i> Axon I	
16:00	Mitsu Ikura (Toronto) Systems Biology of Ras Signalling by NMR	
16:45	Harald Schwalbe (Frankfurt a. M.) NMR in Chemical Biology and Drug Design	
17:30	John-Dylan Haynes (Berlin) What Does Functional MRI Teach us About the Human Mind?	
18:15	Poster Session 2 (even numbers presenting)	
19:30	Barbeque (Poster Session continued)	
20:45	John Waugh and the Early Days of CP	
21:15	Drinks & Dancing	

Thursday, Oct 2, 2014, Campus Buch, MDC.C, Robert-Rössle-Str. 10, 13125 Berlin

	Plenary V: Magnetic Resonance in Structural Biology <i>Chair: Robert Bittl</i> Axon I	
09:00	Anja Böckmann (Lyon) Atomic-Resolution 3D Structure of Amyloid β Fibrils Bearing the Osaka Mutation: Parts I & II	
09:30	Beat Meier (Zurich) Atomic-Resolution 3D Structure of Amyloid β Fibrils Bearing the Osaka Mutation: Parts III & IV	
10:00	Gunnar Jeschke (Zürich) Sensitivity Enhancement in Pulsed EPR on Nitroxide and Gd(III) Spin Labels	
10:30	<i>Coffee Break</i>	
	Plenary VI: Magnetic Resonance in Structural Biology <i>Chair: Thomas Risse</i> Axon I	
11:00	Wayne Hubbell (Los Angeles) Revealing Protein Conformational Substates and Dynamics with Site-Directed Spin Labeling and High Pressure EPR	
11:30	Adam Lange (Berlin) Supramolecular Assemblies Studied by 3D and 4D Solid-State NMR	
12:00	Michael Sattler (Garching) Structure and Dynamics of Protein Complexes Using Integrated Structural Biology	
12:30	Concluding remarks <i>Gerd Buntkowsky, Enrica Bordignon, Thomas Risse, Christina Thiele</i>	
12:40	<i>Lunch (in Campus Mensa)</i>	
13:10	G-NMR	