

Novel Applications of Magnetic Resonance to Condensed Matter

26th Annual Meeting of the Magnetic Resonance Discussion Groups of NMR Discussion Groups of the Society of German Chemists and the Royal Society of Chemistry as well as the British Radio-Frequency Spectroscopy Group

September 28 to 30, 2004
University of Aachen RWTH

Tutorial on
NMR with Spatial Resolution: Methods and Applications
Sept. 27, 2004



Monday, Sept. 27th, 2004

10:00 h – 17:00 h	Tutorial Part: A3, Sammelbau Chemie, Seffent Melaten Campus
10.00 h – 10.15 h	B. Blümich, Aachen: Space Encoding with Pulsed Gradients
10.15 h – 11.35 h	break for coffee
11.35 h – 12.50 h	P. Jakob, Würzburg: Medical Imaging
12.50 h – 14.00 h	break for lunch
14.00 h – 15.15 h	S. Stapf, Aachen: Diffusion and Flow
15.15 h – 15.35 h	Break for coffee
15.35 h – 16.50 h	F. Casanova, Aachen, Mobile NMR
16:00 h – 20:00 h	Registration
19:00h – 21:00 h	Welcome Get together / Executive Board meeting of the German MR Discussion Group in Ibis at Marschiertor ("Soers" room).

Tuesday, Sept. 28th, 2004

8.50 h – 9.05 h	Bernhard Blümich, Duncan Farrant: Opening Remarks Wellcome Address by Prorektor Prof. Dr. Heinen	
9:05 h – 10:45 h	Plenary Lectures: Solids and Materials, Fo2: Bernhard Blümich	
9.05 h – 9.40 h	Malcolm Levitt, Southampton, UK: Symmetry-Based Recoupling: Principles and Applications	
9.40 h – 10.15 h	Hans W. Spiess: Magnetic Resonance: A versatile tool for elucidating nanostructures	
10.15 h – 10:45 h	Joost Lohman, Bruker, UK: Techniques for EPR Imaging	
10:45 h – 11:15 h	Break for Coffee, Karman Auditorium	
11:15 h – 12:35 h	Parallel Sessions	
	Fo2: Pharmaceutical NMR:	Fo3: Solid State NMR I: Klaus
	Herbert Kogler, David Neuhaus	Müller, Robin Harris
11:15 h – 11:35 h	P. Juretschke, Frankfurt, Germany: NMR Spectroscopic Methods in Diabetes and Obesity Research: Characterization of Myocellular Lipid Stores and Their Physiological Role	Julian Griffin, London, UK In vitro, in vivo and in situ NMR studies of glioma: High resolution NMR spectroscopic studies of metabolic compartmentation
11:35 h – 11:55 h	G. Williams, Cambridge, UK: Fragment-Based Drug Design: a synthesis of NMR and X-ray diffraction	Leo van Wüllen, Münster, Germany: A multinuclear solid state NMR study of the network structure in high performance ceramics
11:55 h – 12:15 h	Alfred Ross, Christophe Dhalluin, Hans Senn. Martinsried, Germany: NMR Based Characterization of Different Isoforms of Pegylated Interferon- α : Aspects for Structure Based Quality Control of Protein Batches	David Middleton, Manchester, UK: Solid-state methods for quantitative analysis of drug-target interactions
12:15 h – 12:35 h	Jeremy Nicholson, London, UK: Studying Complex	Christian Jäger, Berlin, Germany: Nanocrystalline

Metabolic System Failure with NMR-based Metabonomics	Biomaterial Hydroxyapatite and its binding in bone: A NMR perspective
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12:35 h – 14:00 h	Break for Lunch (e. g. Mensa or Pontstrasse)
14:00 h – 16:00 h	Plenary Lectures: Liquids, Aula: Duncan Farrant
14:00 h – 14:40 h	Tim Claridge, Oxford, UK: Cyclodextrin rotaxanes: threading, unthreading and shuttling
14:40 h – 15:20 h	Klaus-Peter Dinse, Darmstadt, Germany: High Spin Sensors at Work in Material Science And Chemistry
15:20 h – 16:00 h	Nick Bampos, Cambridge, UK: Probing Non-Covalent Interactions in Supramolecular Assemblies by NMR Spectroscopy
16:00 h – 16:30 h	Break for Coffee, Karman Auditorium
16:30 h – 18:30 h	Poster Session I, Karman Auditorium: Duncan Farrant, Bernhard Blümich
18:30 h – 20:00 h	Break for Dinner (e. g. Pontstrasse, City center)
20:00 h – 21:00 h	Public Evening Lecture devoted to the <i>Year of Technology</i> , Aula: Toni Keller, Rheinstetten, Germany: Kernmagnetische Resonanz: Gestern, Heute und Morgen

Wednesday, Sept 29th, 2004

9:00 h – 10:30 h	Ernst-Prize Awards, Fo2: A. Sebald, D. Neuhaus	
9.00 h – 9.30 h	Bogdan Buhai, Arnold Kühnle, Ioan Ardelean, and Rainer Kimmich, University of Ulm, Germany: Visualization of transport in fluid filled percolation model objects	
9.30 h – 10:00 h	Marina Caravetta, X. Zhao, O. G. Johannessen, W. C. Lai, M. A. Verhoeven, P. H. M. Bovee-Geurts, P. J. E. Verdegem, S. Kiihne, H. Luthman, H. J. M. de Groot, W. J. de Grip, J. Lugtenburg, M. H. Levitt, , Stockholm University, Sweden; Southampton University, UK, Leiden University, The Netherlands, Univeristy of Nijmegen, The Netherlands: Protein-induced bonding perturbation in Rhodopsin studied by DQ solid-state NMR	
10:00 h – 10:30 h	A. Hoffmann, I. Schnell, MPI Folymer Research, Mainz: Two-dimensional double-quantum ² H NMR spectroscopy in the solid state under OMAS conditions: correlating ² H chemical shifts with pseudostatic lineshapes	
10:30 h – 11:00 h	Break for Coffee, Karman Auditorium	
11:00 h – 12:40 h	Parallel Sessions	
	Fo2: High resolution NMR: Methods and Biology, Harald Schwalbe, Jeremy Nicholson	Fo3: Solid Sate NMR II, Angelika Sebald, Malcolm Levitt
11:00 h – 11:25 h	Eric's Kupce, Oxford, UK: Fast Multi-Dimensional NMR Spectroscopy by Projection-Reconstruction	Robin K. Harris, University of Durham, UK, Multinuclear Solid-State Magnetic Resonance Of Tin (II) Compounds
11:25 h – 11:50 h	Hartmut Oschkinat	Ovidiu Andronesi, Gitta Angerstein, Anja Böckmann\$, Stefan Becker, Manuel Etzkorn, Adam Lange, Henrike Heise, Colan E. Hughes, Karsten

		Seidel, and <u>Marc Baldus</u> , Max-Planck-Institute for Biophysical Chemistry, Goettingen, Germany, and Institut de Biologie et Chimie des Protéines, Lyon, France, Studying molecular structure by proton-mediated rare-spin correlation spectroscopy
11:50 h – 12:15 h	David Neuhaus Cambridge, UK: NMR Studies of some DNA-Binding Proteins	Melinda J. Duer, University of Cambridge, UK, How materials combine: solid-state NMR studies of molecular interfaces
12:15 h – 12:40 h	Hans-Robert Kalbitzer, Regensburg, Germany: Automated Structure Determination of Proteins from NMR data	Alia, Leiden Institute of Chemistry and Leiden Institute of Physics, The Netherlands, The electronic and protonic structure of histidines in photosynthetic antenna and reaction centres
12:40 h – 14:00 h	Break for Lunch (e.g. Mensa or Pontstrasse)	
14:00 h – 16:00 h	Parallel Sessions	
	Fo2: Methods and Transport: Stefan Berger, Julian Griffin	Fo3: EPR applications in Biophysics and Material Science: Graham Smith, Robert Bittl
14:00 h – 14:30 h	Philip T. Robinson, Tran N. Pham, <u>Dušan Uhr</u> : The Renaissance of Chemical Shift Selective Filters	Eric J. L. McInnes (13): Multi-frequency EPR of transition metal clusters with high and low spin ground states
14:30 h – 15:00 h	<u>Alexander Fink</u> , Eike Brunner, FEM simulations on the production of hyperpolarized xenon	F. MacMillan: resolving cofactor protein interactions using pulsed EPR spectroscopy
15:00 h – 15:30 h	Simon Duckett (12)	Chris W. M. Kay, Multifrequency EPR and ENDOR studies of photo-active flavoproteins
15:30 h – 16:00 h	<u>Werner Kremer</u> , Norman Kachel, Ralph Zahn, Hans Robert Kalbitzer, Intermediate states and implications for the species barrier of the human prion protein revealed by high pressure NMR	G. Panek, G.P. , S. Schleidt, Q. Mao, G. Jeschke; Structure and dynamics of the inorganic/organic interface in polymer-clay nanocomposites as seen by a multitude of EPR techniques and a dash of NMR
16:00 h – 18:00 h	Break for Coffee and Poster Session II, Karman Auditorium: Duncan Farrant, Bernhard Blümich	
17:30 h – 18:15 h	FGMR Members Meeting, FO3	
18:30 h – 19:45 h	guided city tour	
19:45 h	Bus to the conference dinner	
20:00 h – 23:00 h	Conference Dinner in the Mensa Vita, Melaten Campus	

Thursday, Sept. 30th, 2004

9:00 h – 10:40 h Parallel Sessions

	Fo2: Hyphenated Techniques: Klaus Albert, Tim Claridge	Fo3: Localized NMR: Bernhard Blümich, A. J. Sederman
9:00 h – 9:25 h	<u>B. Bardsley</u> , A.L. Beck, R.D. Farrant, P.J. Moore, GlaxoSmithKline, Stevenage, UK: Practical aspects of LC-SPE-NMR in a pharmacological environment	Rainer Kimmich, University of Ulm, Germany: Electric and hydrodynamic currents through porous media: NMR mapping and comparison
9:25 h – 9:50 h	Hans Hasse, Stuttgart, Germany: High Resolution NMR Spectroscopy in Process Engineering contributed UK	Peter Morris, Nottingham, UK: Exploring the mind with functional magnetic resonance
9:50 h – 10:15 h		R. H. Acosta, L. Agulles-Pedros, P. Blümmler, H. W. Spiess, Mainz, Germany: Optimization of Resolution in Gas MRI
10:15 h – 10:40 h	contributed D	S. Harms, M. Küppers, S. Stapf, B. Blümich, RWTH Aachen, Germany: NMR velocity studies on a fluidized bed
	Fo5: EPR – Photoinduced States and Metalloproteins, A. Thomson, Thomas Prisner	
9:00 h – 9:25 h	Graham M. Smith, St., Andrews, UK: Bringing the NMR paradigm to ESR	
9:25 h – 9:50 h	M. Kaupp	
9:50 h – 10:15 h	contributed GB	
10:15 h – 10:40 h	contributed D	
10:40 h – 11:10 h	Break for Coffee, Karman Auditorium	
11:10 h – 12:30 h	Plenary Lectures: Chemical Engineering, Fo2: Siegfried Stapf, Simon Duckett	
11:10 h – 11:20 h		
11:20 h – 12:00 h	A. J. Sederman, University of Cambridge, UK: Probing unsteady state transport processes using ultra-fast MRI techniques	
12:00 h – 12:40 h	Klaus Albert, University of Tübingen, Germany: Continuous-flow NMR Spectroscopy in Reaction Monitoring	
12:40 h	Conference adjourns	