Tuesday, September 21, 2010

08:30 **Opening** **H. Eckert**

08:35 Presentation of Ernst Awards
H. Kogler (Lecture Hall C1)

08:45 **R. Auer (Wien)** Pharmacophore Mapping via Cross-Relaxation During Adiabatic Fast Passage
09:00 **A. Krahn (Rheinstetten) , M.T. Türke (Göttingen), M. Reese (Göttingen)** Shuttle DNP Spectrometer With a Two Center Magnet
09:15 **M. Roth (Mainz)** Continuous ^{1}H and ^{13}C Signal Enhancement in NMR and MRI Using Parahydrogen and Hollow Fiber Membranes

09:30 **Presentation of C.J. Gorter Award**
P.C.C.M. Magusin (Lecture Hall C1)

09:40 **J. Bart (Nijmegen)** Stripline-Based Microfluidic Devices for High-Resolution NMR Spectroscopy

10:00 **Coffee Break**

1st Plenary Session: Liquid State NMR Methodology
H.R. Kalbitzer (Lecture Hall C1)

10:30 **A. Bax (Bethesda)** Chemical Shifts and Dipolar Couplings: How Can They Help?
11:00 **C. Griesinger (Göttingen)** Fuzzyness of Globular and Aggregating Proteins in Infection and Neurodegeneration: An NMR Spectroscopic View
11.30 **K. Brindle (Cambridge)** Imaging Early Tumour Responses to Therapy Using Magnetic Resonance Imaging and Spectroscopy

12:00 **Lunch**

Parallel Session 1: Advances in Pulsed EPR
T. Prisner (Lecture Hall C 1)

13:30 **G. Jeschke (Zürich)** A Systematic Approach for Characterization of Protein State Transitions by EPR-Derived Distance Constraints
13:55 **S. van Doorslaer (Antwerpen)** Insight in Enantioselective Catalysis via Pulsed EPR and DFT
14:20 **W. Lubitz (Mülheim)** Pulse EPR Techniques Applied to the Metalloenzyme Hydrogenase: Hydrogen Production and Conversion in Nature
14:45 **S. Domingo Köhler (Konstanz)** Analysis of Distance Distributions
15:05 **B. Corzilius (Cambridge)** Novel Concepts in High-Field DNP and Cryogenic MAS NMR

15:25 **Coffee Break**

Parallel Session 2: Liquid State NMR / Small Molecules
J. Martins (Lecture Hall C2)

13:30 **S. Berger (Leipzig)** Lithium: NMR Detection of Weak Interactions
13:55 **D. Jacobs (Vlaardingen)** Nutritional Metabolomics Using ^{1}H NMR Spectroscopy
14:20 **D. Sinnaeve (Gent)** Heteronuclear Relaxation Measurements as a New Method to Study Anisotropic Supramolecular Structures
14:45 **M. Klein (Regensburg)** Discrimination of Steatosis and NASH in Mice Using NMR
15:05 **M. Kunze (Münster)** Ion-Aggregation in Pyrrolidinium-Based Ionic Liquids Probed by NMR Relaxation and PFG-NMR Measurements

15:25 **Coffee Break**

Parallel Session 3: Transport Processes
M. Schönhoff (Lecture Hall C1)

16:00 **S. Stapf (Ilmenau)** Diffusion Exchange Gradients
16:25 **H. van As (Wageningen)** PFG-MRI of Flow, Diffusion and Exchange in Complex Porous Biosystems
16:50 **L. van Lokeren (Paris)** Characterization of Hybrid Core-Shell Star-Like Architectures by Diffusion-Ordered NMR Spectroscopy
17:15 **H.P. Huinink (Eindhoven)** Keeping Track of Water in Thin Polymer Films

Parallel Session 4: Pulsed EPR / DNP Applications
S. van Doorslaer (Lecture Hall C2)

16:00 **R. Bittl (Berlin)** Functional Paramagnetic Inter-mediates in Proteins Studied by *"In-Cell"* EPR
16:25 **A. Pöppl (Leipzig)** Cw and Pulsed EPR Spectroscopy of Paramagnetic Transition Metal Ions in Metal-Organic Framework Compounds
16:50 **M. Huber (Leiden)** EPR Methods for Structure Determination in Biological Systems.
17:15 **P. Lüders (Zürich)** Distance Information in the Nanometer Range Obtained from Ln^{3+} - Nitroxide Radical Spin Pairs

18:00 **Meeting Members of the GDCh-Fachgruppe**
19:00 **Poster session with *Brezeln and Bier***

Wednesday, September 22, 2010

2nd Plenary Session: Sensitivity Enhancement
H. de Groot (Lecture Hall C1)

08:30 **G. Buntkowsky (Darmstadt)** Mechanisms and Applications of Para-Hydrogen Induced Nuclear Polarization in Catalysis and Biomedicine
09:00 **M. Luhmer (Brüssel)** Exploring Photoreactions between Polyazaaromatic Ru(II) Complexes and Biomolecules by Chemically Induced Dynamic Nuclear Polarization Measurements
09:30 **J. Matysik (Leiden)** The Solid-State Photo-CIDNP Effect

10:00 **Coffee Break**

Parallel Session 5: Solid State NMR Methodology
H. Eckert (Lecture Hall C 1)

10:30 **E. Brunner (Dresden)** Solid-State NMR in Biomineralisation: Methodical Challenges and Recent Results
10:55 **M. Baldus (Utrecht)** Solid-State NMR on Complex Biomolecules
11:20 **H. Oschkinat (Berlin)** Structural Investigations on Small Heat Shock Proteins by Solid-State NMR and Adventures with DNP
11:45 **A.P.M. Kentgens (Nijmegen)** NMR Using Small Coils and Large Fields.
12:10 **T. Bräuninger (Stuttgart)** Heteronuclear Spin Decoupling of Quadrupolar Nuclei with Half-Integer Spin in Solid-State NMR

Parallel Session 6: NMR Computation
J. Schmedt auf der Günne (Lecture Hall C 2)

10:30 **A.M.J.J. Bonvin (Utrecht)** Building Macromolecular Assemblies by Information-Driven Docking. Challenges and Perspectives
10:55 **J. Gauss (Mainz)** Interplay of Theory and Experiment in NMR Spectroscopy: Electron-Correlated Calculation of NMR Chemical Shifts
11:20 **M. Kaupp (Würzburg)** Progress in Quantum-chemical Computations: From EPR Parameters of Metallo-enzymes to NMR Shifts of Paramagnetic Systems
11:45 **G.W. Vuister (Nijmegen)** New Tools for NMR Structure Validation
12:10 **F. Mocci (Cagliari)** Fluxional Character of Carboxylates: DFT & ^{17}O NMR Investigations

12:30 **Lunch**

12:30 **Lunch**

Parallel Session 7: Structural Biology (1)
R. Boelens (Lecture Hall C1)

14:00 **H.-R. Kalbitzer (Regensburg)** Static High Pressure NMR Spectroscopy and Multidimensional High Pressure Correlation Spectroscopy of Proteins
14:25 **M. Sattler (Garching)** NMR-Based Structural Analysis of (Large) Protein Complexes in Solution
14:50 **C. Damblon (Liège)** Structural & Dynamic Studies of Metallo-β-Lactamases
15:15 **S. Dames (Garching)** NMR-Characterization of the Membrane-Association of the Redox-Sensitive TOR FATC Domain
15:35 **K. Houben (Utrecht)** NMR Studies of the Yeast Integral Membrane Protein pmp3

Parallel Session 8: Nanomaterials/Interfaces
L. van Wüllen (Lecture Hall C2)

14:00 **P. Heitjans (Hannover)** Dynamics at Interfaces in Nanocrystalline Materials
14:25 **J.C. Martins (Gent)** (Not so) Novel Solution Methods to Study Colloidal Nanoparticles and their Interactions
14:50 **P. Magusin (Eindhoven)** Inorganic Materials for Heterogeneous Catalysis and Energy Storage Investigated with MAS NMR
15:15 **J. Schmedt a. d. Günne (München)** Heteronuclear NMR on Nanoparticles - the Core-Shell Structure by REDOR Experiments
15:35 **A.H. Velders (Enschede)** Let's DENs

15:55 **Coffee Break**

15:55 **Coffee Break**

Parallel Session 9: Metabonomics
J. van Duynhoven (Lecture Hall C1)

16:30 **J.-M. Colet (Mons)** The Hormetic Dose Response in Toxicology as Seen by Metabonomics
16:55 **J. Vervoort (Wageningen)** Automated Identification of Flavonoids
17:20 **W. Kremer (Regensburg)** Single Cell NMR Spectroscopy for the Analysis of Active Transport Processes Across the Plasma Membrane
17:40 **A. Smolinska (Nijmegen)** ^{1}H-NMR Spectroscopy and Pattern Recognition Methods for Metabolomics Investigation of Pre-Clinical Model of Multiple Sclerosis

Parallel Session 10: MR Imaging
M. Verhoye (Lecture Hall C2)

16:30 **R. Muller (Mons)** Magnetic Resonance Molecular Imaging, Reporters and Vectors
16:55 **U. Himmelreich (Leuven)** in vivo Cell Imaging in Animal Models
17:20 **K. Nicolaij (Eindhoven)** The Multifaceted Role of in vivo NMR in Biomedical Research
17:40 **F. Casanova (Aachen)** Halbach Arrays for NMR and MRI

18:30 **Bus transport to Conference Dinner at Café Uferlos**
19:00 **Conference Dinner**

Thursday, September 23, 2010

Parallel Session 11: Catalysis
P. Magusin (Lecture Hall C 1)

08:30 **M. Hunger (Stuttgart)** In situ Solid-State NMR Investigation of the Reactivity of Ethylbenzene in Acidic Zeolites
08:55 **C. Thiele (Darmstadt)** Residual Dipolar Couplings as Novel Restraints for the Structure Determination of Catalytically Active Species
09:20 **R. Willem (Brüssel)** ^{1}H, ^{13}C, ^{119}Sn HRMAS NMR for Monitoring Supported Organotin Catalysts and Catalytic Processes
09:45 **M. Verkuijlen (Nijmegen)** Solid-state NMR Studies of the Local Structure of $NaAlH_4$/C and $LiBH_4$/C Nanocomposites
10:05 **S. Ullrich (Frankfurt/M.)** Interphase Kinetics of an Integral Membrane Kinase by Time-Resolved Solid-state NMR

10:25 **Coffee Break**

Parallel Session 12: Polymers/Complexity
M. Vogel (Lecture Hall C 2)

08:30 **F. Mulder (Groningen)** Determination of Protein Side-Chain Conformations from ^{13}C NMR Chemical Shifts: A Reappraisal of the *gamma-gauche* Effect
08:55 **K. Saalwächter (Halle)** Dynamics in Complex Polymers by High-Resolution Dipolar NMR
09:20 **H. de Groot (Leiden)** Alternating *syn-anti* Bacteriochlorophylls Form Concentric Helical Nanotubes in Chlorosomes and Form the Basis for Supramolecular Light Harvesting Dyes
09:45 **U. Scheler (Dresden)** Polymers under Mechanical Stress
10:05 **G. Brunklaus (Mainz)** Solid-state NMR Studies of Li Ion Mobility in Cyclic Carbonate Based Model Compounds

10:25 **Coffee Break**

3rd Plenary Session: Structural Biology (2)
M. Baldus (Lecture Hall C1)

11:00 **R. Boelens (Utrecht)** Structure and Dynamics in Gene Regulation and DNA Repair
11:30 **H. Schwalbe (Frankfurt/M.)** New Methods for Structure Determination of Proteins and RNA
12:00 **N. van Nuland (Brüssel)** Communication Within and Between Proteins

12:30 **End of Conference**

Monday, September 20, 2010

12:00 **Start registration Conference**

Tutorial: NMR Spectroscopy on Quadrupolar Nuclei (Lecture Hall C2)

14:00 **H. Eckert (Münster)** Nuclear Electric Quadrupolar Interactions in NMR Spectroscopy – An Introduction
14:45 **L. van Wüllen (Münster)** Techniques for Removing Second-Order Quadrupolar Broadening in Solids: From Basic Theory to High Resolution Spectra

15;30 Coffee Break

16:00 **M. Vogel (Darmstadt)** Studies of Molecular Dynamics Using ^{2}H NMR
16:45 **A.P.M. Kentgens (Nijmegen)** Population and Coherence Transfer in Quadrupolar Spin Systems Using Amplitude Modulated Pulses

18:00 Welcome Get Together
19:00 Meeting of the GDCh Executive Committee