EUROISMAR 2019

Sunday, 25 August 2019 - Friday, 30 August 2019

Henry Ford Building

Programme

Sunday 25 August 2019

Registration (10:00-12:30)

Luncheon (12:30-13:00)

Bruker User Meeting (13:00-16:00)

Opening of the Meeting - Max Kade Auditorium (16:00-16:15)

Prize Lectures: Prize Session 1 - Max Kade Auditorium (16:15-18:55)

time	title	presenter
16:15	Introduction of ISMAR Prize	Dr TYCKO, Robert (National Institutes of Health)
16:25	NMR and IDPs	Dr DYSON, Jane (Scripps Research)
16:45	Relaxing with IDPs: NMR analysis of dynamics and molecular interactions	Dr WRIGHT, Peter (Scripps Research)
17:10	Introduction of Ernst Prize	Prof. BANCI, Lucia (CERM-University of Florence (Italy))
17:20	DEER on cells with Gd(III)	Prof. GOLDFARB, Daniella (Weizmann Institute of Science)
17:40	Everyone needs a little help from one’s friends: Synergy between NMR, cryo-EM and large-Scale MD Simulations	Prof. GRONENBORN, Angela M. (University of Pittsburgh School of Medicine)
18:10	Introduction of Felix-Bloch Lecture	Prof. LUY, Burkhard (Institute for Biological Interfaces 4 - Magnetic Resonance and Institute for Organic Chemistry, Karlsruhe Institute of Technology)
18:15	Structure and Dynamics of Membrane Proteins in a Native Environment	Prof. HAGN, Franz (Department of Chemistry and Institute for Advanced Study, Technical University of Munich and Helmholtz Zentrum München)

Welcome Reception (18:55-20:30)

Monday 26 August 2019

Prize Lectures: Prize Session 2 - Max Kade Auditorium (08:40-10:00)

time	title	presenter
08:40	Adventures with Long-Lived States	Prof. LEVITT, Malcolm (University of Southampton)
09:20	New Methods for Dynamic Nuclear Polarization in Insulating Solids: The Overhauser Effect and Time Domain Techniques	Dr CAN, Thach (Massachusetts Institute of Technology)
09:40	Endogenous DNP from Paramagnetic Dopants for Probing Functional Inorganic Materials	Dr LESKES, Michal (Department of Materials and Interfaces, Weizmann Institute of Science)

Coffee - HFB Foyer (10:00-10:30)

EPR: Session 2 - Lecture Hall D (10:30-13:00)

time	title	presenter
10:30	Pulsed EPR and ENDOR with Photonic Bandgap Superconducting Microresonators	Prof. LYON , Stephen (Princeton University)
11:05	Chemical Exchange Processes Studied by 95 GHz 2D-ELDOR	Dr DZIKOVSKI, Boris (Cornell University)
11:30	Tuning Spin Dynamics in Crystalline Tetracene	Dr PANJWANI, Naitik A. (Berlin Joint EPR Lab, Fachbereich Physik, Freie Universität Berlin, D-14195, Berlin, Germany)
11:55	Trityls vs nitroxides as spin labels	Prof. BAGRYANSKAYA, Elena (N.N.Vorozhtsov Institute of Organic Chemistry SB RAS)
12:30	Deep neural network analysis of DEER data	Prof. KUPROV, Ilya (University of Southampton)

In-vivo: Methods: Session 5 - Lecture Hall B (10:30-13:00)

time	title	presenter
10:30	Deuterium Metabolic Imaging (DMI), a novel MR-based method for in vivo mapping of metabolism	Prof. DE GRAAF, Robin (Yale University)
11:05	Quantitative Heterogeneity MRS (qhMRS) - A New Type of Line Shape Analysis Applicable to NMR Resonances Sensitive to Suitable Physicochemical Parameters	Prof. LUTZ, Norbert W. (CRMBM, Aix-Marseille University)
11:30	In-vivo NMR and MRI study of Superparamagnetic Iron Oxide Nanoparticles (SPIONs) on Daphnia Magna	Dr WU, Bing (University of Toronto)
11:55	Imaging Human Brain Metabolism Exploiting Ultra-High Field MRI	Prof. HENNING, Anke (University of Texas Southwestern Medical Center)

12:30	MRI at 2.15 MHz in a large-bore Halbach Array	Prof. WEBB, Andrew (C.J. Gorter Center for High Field MRI, Leiden University Medical Center)

Solution-state NMR Methods: Session 3 - Lecture Hall C (10:30-13:00)

time	title	presenter
10:30	New methods and theory for conformatonal dynamics of macromolecules	Dr PALMER, Arthur (Columbia University)
11:05	Localization of ligands in human carbonic anhydrase by 19F PCS NMR and new lanthanide chelating tags	Dr HÄUSSINGER, Daniel (University of Basel)
11:30	Accurate Measurement of Transverse Relaxation Rates in Systems with Coupled Protons	Dr KIRALY, Peter (University of Manchester)
11:55	Conformation Changes in Proteins Made Visible by Lanthanide Tags	Prof. OTTING, Gottfried (Australian National University)
12:30	De-correlating kinetic and relaxation parameters in exchange saturation transfer NMR	Dr TUGARINOV, Vitali (National Institutes of Health)

Benchtop & Low-field NMR: Session 1 - Max Kade Auditorium (10:30-13:00)

time	title	presenter
10:30	Advances and Adventures with Compact NMR	Prof. BLÜMICH, Bernhard (RWTH Aachen University)
11:05	Understanding novel spin physics to make clinical-scale hyperpolarization simple, fast and cheap	Prof. WARREN, Warren (Duke University)
11:30	Compact NMR for Metabolic Health Screening and Diabetes Prevention	Prof. CISTOLA, David (Texas Tech University Health Sciences Center El Paso)
11:55	A MOUSE for Heritage: In Pursuit of Art and Culture	Prof. BAIAS, Maria (New York University Abu Dhabi)
12:30	Wide field range studies of nuclear magnetic relaxation using optically pumped magnetometers	Mr BODENSTEDT, Sven (ICFO)

Biomolecules: IDP: Session 4 - Lecture Hall A (10:30-13:00)

time	title	presenter
10:30	Disordered Protein Complexes	Prof. KRAGELUND, Birthe B. (University of Copenhagen)
11:05	Cross-correlated relaxation for studying intrinsically disordered proteins	Dr ZAWADZKA-KAZIMIERCZUK, Anna (University of Warsaw)
11:30	NMR insight into transient structures and interactions within the RNA polymerase of bronchiolitis virus	Dr SIZUN, Christina (CNRS, Institut de Chimie des Substances Naturelles)
11:55	The role of proline residues in intrinsically disordered proteins	Prof. PIERATTELLI, Roberta (CERM, University of Florence)

12:30	The NMR structure of a gp41 cytoplasmic tail fragment reveals the structural basis of the transmembrane coupling of the HIV-1 envelope glycoprotein	Dr PIAI, Alessandro (Harvard Medical School)

Lunch (13:00-14:00)

Posters: odd numbered presentations (14:00-16:00)

Coffee (16:00-16:15)

Materials: Session 6 - Lecture Hall A (16:15-17:40)

time	title	presenter
16:15	Probing Ion Mobility Mechanisms in Solid Electrolytes using Solid-State NMR	Dr JOHNSTON, Karen (Durham University)
16:50	Structure and Dynamics of Defects in Metal-organic Frameworks studied by Solid-state NMR	Ms FU, Yao (Zhejiang University)
17:15	Solid-state and in situ NMR studies of flexible metal-organic frameworks	Prof. BRUNNER, Eike (TU Dresden)

Biomolecules: Membranes: Session 8 - Max Kade Auditorium (16:15-17:40)

time	title	presenter
16:15	New Long-Distance SSNMR Techniques and Their Applications to Protein Structure Determination	Prof. HONG, Mei (MIT)
16:50	Molecular mechanisms behind Remorin nanodomain formation	Dr HABENSTEIN, Birgit (CBMN / IECB UMR 5248 CNRS University of Bordeaux)
17:15	Solution NMR of nanodisc-embedded proteins: new molecular insights into protein-protein and protein-membrane interactions	Prof. CHILL, Jordan (Department of Chemistry, Bar Ilan University)

Biomolecules: Modelling of Biological Processes: Session 7 - Lecture Hall C (16:15-17:40)

time	title	presenter
16:15	Copper trafficking in eukaryotic systems: Current knowledge from experimental and computational efforts	Prof. RUTHSTEIN, Sharon (Bar Ilan University)
16:50	Structural description of the target search process by a disordered transcription factor	Mr KELLY, Conor (University of Oxford)
17:15	A generalized approach for NMR studies of lipid–protein interactions based on sparse fluorination of acyl chains	Dr DIERCKS, Tammo (CiC bioGUNE)

Biomolecules: Carbohydrate Interactions: Session 9 - Lecture Hall D (16:15-17:40)

time	title	presenter
16:15	Selective High-Resolution DNP-Enhanced NMR of Biomolecular Binding Sites	Dr HEDIGER, Sabine (CNRS)
16:50	Interaction between Cell-Wall and Biosynthetic Enzymes Using a Combination of Liquid- and Solid-State NMR Approaches	Prof. SIMORRE, Jean-Pierre (CNRS)
17:15	Unravelling Glycan-Lectin Interactions: from STD to Paramagnetic NMR	Prof. JIMENEZ-BARBERO, Jesus (CIC bioGUNE)

Spin Physics: Session 10 - Lecture Hall B (16:15-17:40)

time	title	presenter
16:15	Electron Spin Relaxation Mechanisms of Atomic Hydrogen Trapped in Silsesquioxane Cages: the Role of Isotope Substitution	Dr MITRIKAS, George (Institute of Nanoscience and Nanotechnology, NCSR Demokritos)
16:50	Coherent control of solid state nuclear spin nano-ensembles	Dr NAYDENOV, Boris (Institute for Nanospectroscopy, Helmholty Zentrum Berlin für Materialien und Energie, Kekulestr. 5, 12489 Berlin)
17:15	Stable radicals tethered to pentacene studied using time resolved EPR and transient absorption spectroscopy	Dr AVALOS, Claudia E. (Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne)

Plenary Lectures - Max Kade Auditorium (17:40-18:30)

time	title	presenter
17:40	Summarizing the static DNP mechanisms	Prof. VEGA, Shimon (Weizmann Institute of Science)

Bruker Night (18:30-21:00)

Tuesday 27 August 2019

Plenary Lectures - Max Kade Auditorium (08:40-10:00)

time	title	presenter
08:40	Magnetic resonance for Cellular Structural Biology: from protein structures to functional processes in a cellular context	Prof. BANCI, Lucia (CERM and Dept. of Chemistry, University of Florence)
09:20	Diffusion and electrophoretic NMR to characterize ion transport in electrolytes	Prof. SCHÖNHOFF, Monika (Institute of Physical Chemistry, University of Muenster)

Coffee (10:00-10:30)

Hyperpolarization: Techniques: Session 12 - Lecture Hall D (10:30-13:00)

time	title	presenter
10:30	Confining and Quantifying Hyperpolarization: 460 GHz-700 MHz DNP NMR using Closed-Cycle Helium MAS and Dual Gyrotron Setup	Dr MATSUKI, Yoh (Osaka University)
11:05	Multi-Sample Dissolution DNP with a Cryogen-Free Polariser	Dr GAUNT, Adam (University of Cambridge)
11:30	Catalyzing the progress in parahydrogen-based NMR hyperpolarization	Prof. KOPTYUG, Igor V. (International Tomography Center, SB RAS)
11:55	Utilizing hyperpolarized noble gas T1 relaxation contrast for MRI in biomedical and engineering applications.	Prof. MEERSMANN, Thomas (University of Nottingham)
12:30	75% Liquid-State 1H Polarization for Hyperpolarized Water	Dr PINON, Arthur C. (Technical University of Denmark)

Dynamics: Session 13 - Lecture Hall A (10:30-13:00)

time	title	presenter
10:30	Allostery and Dynamics in Ion Channels and Oligomeric Proteins	Prof. MCDERMOTT, Ann (Columbia University)
11:05	A high-resolution description of functional dynamics and allosteric coupling of the β1-adrenergic receptor from backbone NMR	Dr GRAHL, Anne (Biozentrum, University of Basel, Switzerland)
11:30	13C-detected NMR methods to characterise side-chain behaviour in large molecular systems	Dr PRITCHARD, Ruth B. (University of Sussex)
11:55	Inspection of solution-state NMR data to evaluate protein conformational changes	Dr ISHIMA, Rieko (University of Pittsburgh School of Medicine)
12:30	Lanthanide-induced relaxation anisotropy	Dr SUTURINA, Elizaveta (University of Bath)

Biomolecules: Session 14 - Max Kade Auditorium (10:30-13:00)

time	title	presenter

10:30	NMR investigation of the activation mechanism of the guardian of the germ cell TAp63a	Prof. DÖTSCH, Volker (Goethe University)
11:05	Flavivirus capsid assembly and dynamics: evidence of a structure-driven regulation of protein interaction with intracellular hydrophobic interfaces.	Prof. ALMEIDA, Fabio C. L. (Federal University of Rio de Janeiro (UFRJ))
11:30	Progress of the structural characterization on a eukaryotic rhodopsin by solid-state NMR	Prof. WANG, Shenlin (Peking University)
11:55	Insights into the Antifungal Activity of Amphotericin B from Solid-State NMR	Prof. RIENSTRA, Chad M. (University of Illinois at Urbana-Champaign)
12:30	Assessing site-specific water accessibility in folded and unfolded proteins using hyperpolarization-enhanced 2D HMQC NMR	Prof. FRYDMAN, Lucio (Department of Chemical and Biological Physics, Weizmann Institute of Science)

Computation: Session 11 - Lecture Hall B (10:30-13:00)

time	title	presenter
10:30	Splitting hairs: Small physical effects in NMR	Prof. VAARA, Juha (University of Oulu)
11:05	Second order dispersion by optimised rotation pulses	Dr GOODWIN, David (Karlsruhe Institute of Technology)
11:30	First-principles computations of NMR shifts for extended paramagnetic solids: significant effects beyond the contact shifts	Dr MONDAL, Arobendo (Technical University of Munich, Germany)
11:55	Computational methods for NMR crystallography of zeolites	Prof. BROUWER, Darren (Redeemer University College)
12:30	Methionine renaissance: computing methyl NMR assignments from X-ray structures	Prof. PONS, Miquel (University of Barcelona)

Materials: Session 15 - Lecture Hall C (10:30-13:00)

time	title	presenter
10:30	Defects within Solid Materials Elucidated using NMR Spectroscopy – from Local Vacancies to Mesoscale Disorder	Prof. SENKER, Juergen (University of Bayreuth)
11:05	125Te broadband solid-state NMR of the Dirac edge states in ultrathin Bi$_{2}$Te$_{3}$ nanoplatelets	Mr PAPAWASSILIOU, Wassilios (Department of Materials and Environmental Chemistry,Stockholm University)
11:30	Transport of Organic Electrolytes and Ionic Liquids in Carbon Materials for Supercapacitors: The High-Gradient NMR Approach	Dr DVOYASHKIN, Muslim (Institute of Chemical Technology, Universität Leipzig)
11:55	Solid-state NMR studies of the electrochemical cycling of LiNi$_{0.8}$Mn$_{0.1}$Co$_{0.1}$O$_2$ cathodes	Dr MÄRKER, Katharina (University of Cambridge; The Faraday Institution)

12:30	Surface Structure Determination of Heterogeneous Catalysts by DNP SENS	JABBOUR, Ribal (High-Field NMR Center, Université de Lyon, FRE 2034, CNRS/ENS Lyon/ UCB Lyon1)

Lunch (13:00-14:00)

Posters: odd numbered presentations (14:00-16:00)

Coffee (16:00-16:15)

Instrumentation: Session 19 - Lecture Hall D (16:15-17:40)

time	title	presenter
16:15	Dissolvable inserts for achieving performance enhanced resonators	Prof. MARTIN, Rachel (University of California, Irvine)
16:50	Rapid scan EPR-on-a-chip	KÜNSTNER, Silvio (Berlin Joint EPR Laboratory, Institut für Nanospektroskopie, Helmholtz-Zentrum Berlin für Materialien und Energie)
17:15	Rheology and 23Na Multiple Quantum Filtered (MQF) rheo-NMR and MRI of Bile Salt Micelles	Dr PAVLOVSKAYA, Galina (University of Nottingham)

Small Molecules: Session 16 - Lecture Hall B (16:15-17:40)

time	title	presenter
16:15	New approaches for J-coupling measurement and five-membered ring conformation analysis	Dr SINNAEVE, Davy (CNRS / Université de Lille)
16:50	A boost in Drug Discovery with Secondary-labeled Hyperpolarized Ligands	Dr CALA, Olivier (Université de Lyon, Université Claude Bernard Lyon 1, ENS de Lyon, CNRS, CRMN FRE 2034)
17:15	Monitoring Oxygen Levels in Microfluidic Devices using 19F NMR	Ms OSTROWSKA, Sylwia (University of Southampton)

NMR in Drug Design: Session 20 - Max Kade Auditorium (16:15-17:40)

time	title	presenter
16:15	Cancer Drug Discovery Using Fragment-Based Methods and Structure-Based Design	Prof. FESIK, Stephen (Vanderbilt University School of Medicine)
16:50	Modulation of aggregating proteins studied by NMR and beyond in neuro- and cellular degeneration	Prof. GRIESINGER, Christian (MPIbpc)
17:15	NMR as a tool for defining cyclotide membrane binding: applications in medicine and agriculture	Prof. CRAIK, David (University of Queensland)

EPR: Session 17 - Lecture Hall C (16:15-17:40)

time	title	presenter
16:15	Studying structure and function of sialic acid TRAP transporters from pathogenic bacteria by pulsed EPR, FRET and X-ray crystallography	Dr HAGELUEKEN, Gregor (University of Bonn)
16:50	When stronger magnets don’t help: Methods for disentangling overlapping high-field EPR spectra illustrated in record organic solar cell blend PBDB-T:ITIC	Ms VAN LANDEGHEM, Melissa (Department of Physics, University of Antwerp)
17:15	Non-magnetic magnetic resonance	Prof. JESCHKE, Gunnar (ETH Zürich)

Biomolecules: Phase Separation: Session 18 - Lecture Hall A (16:15-17:40)

time	title	presenter
16:15	Conformations of Tau in Dynamic Assemblies	Prof. ZWECKSTETTER, Markus (German Center for Neurodegenerative Diseases (DZNE))
16:50	Multivalency and phase separation of measles virus replication machinery.	GUSEVA, Serafima (Viral Replication Machines Group & Protein Dynamics and Flexibility by NMR Group, Institut de Biologie Structurale (IBS), CEA, CNRS, University Grenoble Alpes, Grenoble, France)
17:15	A Molecular View of the Liquid to Gel Phase Transition of Heterochromatin Protein HP1α	Prof. DEBELOUCHINA, Galia (University of California, San Diego)

Plenary Lectures - Max Kade Auditorium (17:40-18:25)

time	title	presenter
17:45	Transporter Conformational Dynamics from Spin Labeling EPR Spectroscopy	Prof. MCHAOURAB, Hassane S. (Vanderbilt University)

Society Meetings: AMPERE General Assembly - Max Kade Auditorium (18:25-18:55)

Posters: even numbered presentations (19:00-21:00)

Wednesday 28 August 2019

Plenary Lectures - Max Kade Auditorium (08:40-10:00)

time	title	presenter
08:40	Recent Developments of DNP Enhanced Solid-State NMR Spectroscopy at High Magnetic Field and Fast MAS	Prof. LESAGE, Anne (University of Lyon)
09:20	Boosting clinical diffusion MRI with principles from solid-state and Laplace NMR	Prof. TOPGAARD, Daniel (Lund University)

Coffee (10:00-10:30)

EPR: Session 22 - Lecture Hall D (10:30-12:30)

time	title	presenter
10:30	ESR microfluidics with picoliter samples	Prof. BLANK, Aharon (Technion - Israel Institute of Technology)
11:05	Spin-labeled nanobodies as proteins' conformational reporters towards in-cell EPR applications.	Dr GALAZZO, Laura (Ruhr University Bochum)
11:30	Quantitative sub-micromolar pulse dipolar EPR spectroscopy evidences high copper(II) labeling efficiency for double-histidine motifs	Dr BODE, Bela (University of St Andrews)
11:55	High-Frequency Electron-Nuclear Double Resonance to Study Biomolecules	Prof. BENNATI, Marina (MPI for Biophysical Chemistry & University of Göttingen)

Instrumentation: Session 25 - Lecture Hall A (10:30-12:30)

time	title	presenter
10:30	Wither the Spin Diffusion Barrier	Prof. GRIFFIN, Robert G. (MIT)
11:05	Squeeze It Until It Breaks: In-situ NMR at Geophysically Relevant Conditions	Dr MEIER, Thomas (Bavarian Geoinstitute)
11:30	Microscale NMR-spectroscopy with femtomole sensitivity using diamond quantum sensors	Dr BUCHER, Dominik (Technical University of Munich)
11:55	Solid State NMR Probes for 1.5 GHz Spectrometer	Prof. GOR'KOV, Peter (National High Magnetic Field Laboratory)

Biomolecules: Integrated Structural Biology: Session 23 - Max Kade Auditorium (10:30-12:30)

time	title	presenter
10:30	Integrative structural biology of non-coding RNA-protein complexes: telomerase and 7SK	Prof. FEIGON, Juli (University of California Los Angeles)
11:05	A Case of Domain Cooperation in a Multidomain Protein Interaction at Telomeres.	Dr CUNIASSE, Philippe (Institute for Integrative Biology of the Cell (I2BC), CEA, CNRS, Université Paris-Saclay)

11:30	Solution structure of Upstream-of-N-Ras, a 116 kDa multi-domain RNA binding protein	Dr HENNIG, Janosch (Structural and Computational Biology Unit, EMBL Heidelberg)
11:55	High molecular-weight complexes in the regulation of gene expression: a view by integrative structural biology	Prof. CARLOMAGNO, Teresa (Leibniz Universität Hannover)

Small Molecules: Session 21 - Lecture Hall B (10:30-12:30)

time	title	presenter
10:30	Boosting the NMR characterization of small- to medium-sized molecules	Prof. E. KÖVÉR, Katalin (University of Debrecen)
11:05	Prebiotic Organization of Biomolecules on Mineral surfaces	Mr ABADIAN, Hagop
11:30	Recent advances in polypeptidic thermoresponsive alignment media for organic compounds	Prof. THIELE, Christina M. (Technische Universität Darmstadt)
11:55	Fast quantitative 2D NMR for metabolomics	Prof. GIRAUDEAU, Patrick (Université de Nantes)

Biomolecules: Molecular Chaperones: Session 24 - Lecture Hall C (10:30-12:30)

time	title	presenter
10:30	The True Tales of the Flexible Tails – Interaction of J-domain Protein with Hsp70 chaperones	Dr ROSENZWEIG, Rina (Weizmann Institute of Science)
11:05	Dynamic regulation of human Hsp70 chaperone functional cycle by its co-chaperones and client protein	Dr MAS, Guillaume (Biozentrum, University of Basel)
11:30	NMR Informed Molecular Modeling to Capture Transient Chaperone-Substrate Interactions	Dr SALMON, Loic (Centre de RMN à Très Hauts Champs (CNRS/ENSL/UCBL))
11:55	Atomic Insight into the Function and Activity of Molecular Chaperones	Dr KALODIMOS, Charalampos (St Jude Children's Research Hospital)

Brunch (12:30-13:30)

Prize Lectures: GDCh Prize Lectures - Max Kade Auditorium (13:30-14:20)

time	title	presenter
13:35	Complex Formation of the Tetracycline□Binding Aptamer Investigated by Specific Cross□Relaxation under DNP	ALADIN, Victoria (Goethe University Frankfurt)
13:45	Insight into small molecule binding to the neonatal Fc receptor by X-ray crystallography and 100 kHz magic-angle-spinning NMR	FRIEDRICH, Daniel (Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany)
13:55	Time evolution of coupled spin systems in a generalized Wigner representation	Dr KOCZOR, Bálint (Technische Universität München, now University of Oxford)

14:05	Dynamic nuclear polarization of 13C in the liquid state over a 10 Tesla field range	Dr ORLANDO, Tomas (RG ESR Spectroscopy, Max Planck Institute for Biophysical Chemistry)

Plenary Lectures - Max Kade Auditorium (14:20-15:00)

time	title	presenter
14:20	Stronger Together: Bacterial Weaving of Functional Amyloid and Polysaccharide Composites to Assemble Multicellular Biofilm Communities	Prof. CEGELSKI, Lynette (Stanford University)

Tutorials - Max Kade Auditorium (15:00-18:00)

time	title	presenter
15:00	Basics of MRI	ITTERMANN, Bernd (Physikalisch-Technische Bundesanstalt (PTB))
16:00	Quantum-Chemical Methods	Prof. KAUPP, Martin (Technische Universität Berlin)
17:00	You Spin Me Right 'Round: Tensors and Rotations in NMR	Prof. MUELLER, Leonard (UC Riverside)

Society Meetings: GDCh Members' Meeting - Lecture Hall C (15:15-16:15)

Music - Lecture Hall A (18:10-19:40)

Thursday 29 August 2019

Plenary Lectures - Max Kade Auditorium (08:40-10:10)

time	title	presenter
08:40	Optically-pumped dynamic nuclear polarization under ambient conditions via nitrogen-vacancy centers in diamond	Prof. MERILES, Carlos (CUNY - CIty College of New York)
09:30	High-resolution NMR spectroscopy applied for field inhomogeneity and spectral congestion	Prof. CHEN, Zhong (Xiamen University) Prof. HUANG, Yuqing (Department of Electronic Science, Xiamen University, Xiamen, China)

Society Meetings: ISMAR General Assembly - Max Kade Auditorium (09:20-09:30)

Coffee (10:10-10:30)

Metabolomics: Session 27 - Lecture Hall B (10:30-13:00)

time	title	presenter
10:30	New Discoveries on HBV infection by Metabolomics	Prof. WANG, Yulan (Singapore Phenome Center, Lee Kong Chian School of Medicine, Nanyang Technological University)
11:05	Slice-selective, high-resolution MAS NMR of intact tissue biopsies gives improved spatial resolution of metabolic distributions	Ms VONHOF, Elisabeth V. (Division of Integrative Systems and Digestive Medicine, Department of Surgery and Cancer, Imperial College London)
11:30	Advanced Analysis of Chronic Kidney Disease by NMR Derived Metabolomic Fingerprints	Prof. GRONWALD, Wolfram (Institute of Functional Genomics, University of Regensburg, Germany)
11:55	Improving survival predictability and biological insight through NMR based metabolomics of Acute Respiratory Distress Syndrome (ARDS)	Dr SINHA, Neeraj (Centre of Biomedical Research)
12:30	The effect of osmolytes in biomolecular stability as investigated by NMR spectroscopy. Lessons from halophilic proteins	Dr MILLET, Oscar (CIC bioGUNE)

Biomolecules: Session 28 - Lecture Hall C (10:30-13:00)

time	title	presenter
10:30	Spinning faster: Developments and Applications to Biological NMR	Prof. MEIER, Beat H (ETH Zurich)
11:05	Sensitivity-Enhanced Protein Solid-state NMR using Ultra-fast MAS and Structural Studies of Alzheimer's Amyloid-β	Dr ISHII, Yoshitaka (Tokyo Institute of Technology)
11:30	Atomic resolution characterization of a folding intermediate by pressure-jump NMR	Dr CHARLIER, Cyril (NIH)

11:55	Monitoring phosphorylation events at the interface between the nuclear envelope and chromatin	Dr ZINN-JUSTIN, Sophie (Institute for Integrative Biology of the Cell, CEA, CNRS, Université Paris-Saclay, CE-Saclay, Gif/Yvette, France)
12:30	Protein phase diagrams determined by high-pressure NMR	Prof. BALBACH, Jochen (Martin-Luther-University Halle-Wittenberg)

In-vivo: In-cell NMR: Session 29 - Max Kade Auditorium (10:30-13:00)

time	title	presenter
10:30	In-Cell NMR: Past, Present and Future	Prof. SELENKO, Phil (Weizmann Institute of Science)
11:05	In-cell PELDOR of spin-labelled RNA duplexes	Dr COLLAUTO, Alberto (Institute of Physical and Theoretical Chemistry and Center for Biomolecular Resonance)
11:30	In-cell DNP Supported Solid-State NMR on Soluble Proteins	Mr NARASIMHAN, Siddarth (Utrecht University)
11:55	Structure determination of antimicrobial peptides in model membranes and live bacteria	Prof. SEPAROVIC, Frances (University of Melbourne)
12:30	Fluxomic studies by in cell and in vitro Dissolution-Dynamic Nuclear Polarization NMR	Mr GUARIN, David (Laboratoire des biomolécules, LBM, Département de chimie, École normale supérieure, PSL University, Sorbonne Université, CNRS, 75005 Paris, France)

Hyperpolarization in Materials: Session 26 - Lecture Hall A (10:30-13:00)

time	title	presenter
10:30	Dynamic Phenomena in Fuel Cells and Batteries Investigated by Various NMR Techniques	Dr HAN, Oc Hee (Korea Basic Science Institute)
11:05	Bulk Hyperpolarization of Inorganic Materials	BJÖRGVINSDÓTTIR, Snaedis (EPFL)
11:30	Room-temperature triplet dynamic nuclear polarization in nanoporous materials and in water	Prof. YANAI, Nobuhiro (Kyushu University)
11:55	DNP Polarizing Agents for High-Field, Fast-MAS and Variable Temperature	Prof. LELLI, Moreno (University of Florence)
12:30	Improving bis-nitroxides' geometry for MAS-DNP	MENTINK-VIGIER, Frederic (National High Magnetic Field Laboratory, Florida State University)

Solid-state NMR Methods: Session 30 - Lecture Hall D (10:30-13:00)

time	title	presenter

10:30	High-Field and Fast-MAS Solid-State NMR: Enabling Application to Pharmaceuticals and Supramolecular Assembly	Prof. BROWN, Steven (University of Warwick)
11:05	Protein resonance assignment without spectral analysis: five-dimensional spectroscopy of immobilized proteins at ultrafast MAS	Dr STANEK, Jan (Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw)
11:30	Solid-state NMR strategies towards speed and resolution	Ms SHARMA, Kshama (TIFR Centre for Interdisciplinary Sciences)
11:55	Multiple acquisitions for protein assignment, structure and dynamics	Prof. LEWANDOWSKI, Józef (University of Warwick)
12:30	Biomolecular structural conversion processes probed with DNP-enhanced, millisecond time-resolved solid state NMR	Dr TYCKO, Robert (National Institutes of Health)

Lunch (13:00-14:00)

Posters: even numbered presentations (14:00-16:00)

Coffee (15:50-16:10)

EPR: Session 31 - Lecture Hall C (16:10-17:15)

time	title	presenter
16:10	Muti-Extreme THz ESR -Recent Developments and Future-	Prof. OHTA, Hitoshi (Kobe University, Molecular Photoscience Research Center)
16:45	High-Q Photonic Band Gap Resonators for mm-wave EPR of Lossy Aqueous Samples and Thin Films	Prof. SMIRNOV, Alex (North Carolina State University)

Metabolomics: Methods: Session 34 - Max Kade Auditorium (16:10-17:15)

time	title	presenter
16:10	A Tale of Two Sugars: 13C NMR Tracking of the Metabolic Fates of Glucose and Fructose in Cancer	Prof. LUMATA, Lloyd (University of Texas at Dallas)
16:45	Metabolic Pathway Profiling (MPP) with stable-isotope tracing	Dr LUDWIG, Christian (University of Birmingham)

Biomolecules: Nucleic Acids: Session 33 - Lecture Hall B (16:10-17:15)

time	title	presenter
16:10	Guanine-rich DNA regions and their amazing structures	Prof. PLAVEC, Janez (Slovenian NMR Center, National Institute of Chemistry, Ljubljana, Slovenia, Slovenia)
16:45	Unique quadruplex structure and anti-disease activity of RNA aptamer, and in-cell NMR of nucleic acids	Prof. KATAHIRA, Masato (Kyoto University)

In-vivo: Session 35 - Lecture Hall A (16:10-17:15)

time	title	presenter
16:10	Imaging Human Brain Function and Connectivity over Multiple Spatial Scales	Prof. UGURBIL, Kamil (University of Minnesota)
16:45	Deuterium Metabolic Imaging for in-vivo monitoring of pregnancy in mice at 15.2 T.	Dr MARKOVIC, Stefan (Weizmann Institute of Science, Department of Chemical and Biological Physics, Rehovot, Israel)

Spin Physics: Session 32 - Lecture Hall D (16:10-17:15)

time	title	presenter
16:10	Up-conversion of NMR signals from radio-frequency to optical regimes through a mechanical transducer	Dr TAKEDA, Kazuyuki (Kyoto University)
16:45	Algorithmic cooling by using long-lived singlet states	RODIN, Bogdan (International Tomography Center)

Plenary Lectures - Max Kade Auditorium (17:15-17:55)

time	title	presenter
17:15	Pulsed magnetic resonance with a free-electron laser	Prof. SHERWIN, Mark (University of California at Santa Barbara)

Conference Banquet (19:00-21:30)

Friday 30 August 2019

Plenary Lectures - Max Kade Auditorium (08:40-10:00)

time	title	presenter
08:40	NMR of Aromatic Side Chains in Large Proteins	Prof. WAGNER, Gerhard (Harvard Medical School)
09:20	Manipulation of Spin Dynamics for Extraction of Spectral Parameters, Ultra High Resolution and Sensitivity Enhancement: Application to small molecules	Prof. SURYAPRAKASH, Nagaraja rao (Indian Institute of Science)

Coffee (10:00-10:30)

Hyperpolarization: Session 39 - Lecture Hall A (10:30-12:30)

time	title	presenter
10:30	High Throughput Hyperpolarization for Drug Screening	Prof. BODENHAUSEN, Geoffrey (Ecole Normale Supérieure)
11:05	Frequency-Chirped Millimeter-Wave Control of 13C-DNP in Diamond	Dr SHIMON, Daphna (Dartmouth College)
11:30	Signal-improved real-time NMR spectroscopy of proteins by hyperpolarized water	Prof. KURZBACH, Dennis (University of Vienna)
11:55	SABRE Chemistry and Spin Physics for High Precision Measurements and Biomedical Applications	Dr LEHMKUHL, Sören (North Carolina State University)

MRI Developments: Session 37 - Lecture Hall B (10:30-12:30)

time	title	presenter
10:30	Developments of NMR for Applications in Chemical Engineering and Medicine	Prof. GALVOSAS, Petrik (MacDiamid Institute for Advanced Materials and Nanotechnology, School of Chemical and Physical Sciences, Victoria University Wellington)
11:05	New developments in production of proton-hyperpolarized propane gas for MRI	Dr SALNIKOV, Oleg G. (International Tomography Center SB RAS and Novosibirsk State University)
11:30	Ultra-high field MRI and MRS: Opportunities and Challenges from Anatomical Imaging and Metabolite Detection for Biological Specimens	Ms KRUG, Julia R. (Laboratory of BioNanoTechnology and Laboratory of Biophysics,Wageningen University & Research)
11:55	In vivo three-dimensional extracellular pH mapping of tumors using EPR	Prof. HIRATA, Hiroshi (Hokkaido University)

Solution-state NMR Methods: Session 40 - Max Kade Auditorium (10:30-12:30)

time	title	presenter

10:30	Investigating the dynamic conformational landscape of G-protein-coupled receptors (GPCRs)	Dr NIETLISPACH, Daniel (University of Cambridge, Department of Biochemistry)
11:05	Light-induced changes in the conformational dynamics of a reversibly photo-switchable fluorescent protein revealed by solution NMR spectroscopy	Ms CHRISTOU, Nina-Eleni (Institute de Biologie Structurale, UGA, CNRS, CEA)
11:30	Ribosome induced riboswitch structure melting	Mrs DE JESUS, Vanessa (Goethe University Frankfurt am Main)
11:55	Leveraging the Achilles heel of high-gamma nuclei to observe low-gamma nuclei.	Dr ARTHANARI, Haribabu (Havard Medical School)

Spin Physics: Session 36 - Lecture Hall C (10:30-12:30)

time	title	presenter
10:30	Ultrasensitive beta-detected NMR at CERN: first results in physics and biology	Prof. KOWALSKA, Magdalena (UNIGE, CERN)
11:05	Direct magnetic field dependence of NMR shielding	Dr KANTOLA, Anu M. (University of Oulu)
11:30	Towards single-shot readout of NV centers in diamond by low-temperature spin-to-charge conversion	Dr REINHARD, Friedemann (TU München, Walter Schottky Institut)
11:55	Magnetic Resonance Spectroscopy of A Single Molecule	Prof. SHI, Fazhan (University of Science and Technology of China)

Dynamics: Session 38 - Lecture Hall D (10:30-12:30)

time	title	presenter
10:30	Allosteric signaling pathways and energetics in the glucocorticoid receptor	Prof. AKKE, Mikael (Lund University)
11:05	Rheological NMR for the study of polymer dynamics	Dr SCHELER, Ulrich (Leibniz-Institut für Polymerforschung Dresdne e.V.)
11:30	Molecular ordering and dynamics in anisotropic soft materials studied by low-resolution proton NMR	Prof. SAALWÄCHTER, Kay (Martin-Luther-Univ. Halle-Wittenberg)
11:55	Extending the range of magnetic fields for high-resolution biomolecular NMR by orders of magnitude	Prof. FERRAGE, Fabien (CNRS and Ecole Normale Superieure)

Brunch (12:30-13:30)

Awards Session - Max Kade Auditorium (13:30-14:10)

Suraj Manrao Student Poster Awards, FEBS Journal Poste Awards, Wiley Awards, JMR Awards

Plenary Lectures - Max Kade Auditorium (14:10-15:30)

time	title	presenter
14:10	Nanoscale magnetic spin resonance using the nitrogen vacancy centre in diamond	Prof. HOLLENBERG, Lloyd C. L. (School of Physics, University of Melbourne, Australia)
14:50	Dynamic Complexes and Complex Dynamics - NMR Studies of Large Scale Protein Motions	Dr BLACKLEDGE, Martin (Protein Dynamics and Flexibility by NMR)

Closing Remarks - Max Kade Auditorium (15:30-15:50)