

Scientific Programme

Monday, September 09, 2024

Lab Tour

10.00 a.m **In-situ spectroscopy @LIKAT**

Leibniz-Institut für Katalyse e.V.
Albert-Einstein-Str. 29

Open Doors

12.00 p.m **MRI Flow Lab**

MRI Flow Lab
Albert-Einstein-Str. 2

Tutorials

Chair: G. Mathies

Arno-Esch-Lecture Hall 1

- 03.00 p.m **In-situ and Operando EPR as a Tool in Catalysis Research**
T. Risse, Berlin/DE
- 04.00 p.m **Basics of Magnetic Resonance Imaging and Flow MRI**
S. Grundmann, Rostock/DE
- 05.00 p.m **Machine Learning: the simple algebra behind the hype**
I. Kuprov, Southampton/GB

Welcome & Awards

Chair: J. Matysik

Audimax

- 06.00 p.m **Conference Opening** - B. Corzilius
- 06.30 p.m **Felix Bloch Lecture** - J. Behrends
- 07.30 p.m Welcome Mixer

Scientific Programme

Tuesday, September 10, 2024

Plenary Session

Chair: T. Prisner

Audimax

- 08.30 a.m **Deciphering the dynamic nature of essential cellular machineries – lessons learned from in vitro and in situ NMR spectroscopy**
B. M. Burmann, Gothenburg/SE
- 09.00 a.m **Rapid scan ESR: A Versatile Tool for the Spin Relaxation Studies at (sub)THz Frequencies**
P. Neugebauer, Brno/CZ, O. Laguta, Brno/CZ, M. Sedivy, Brno/CZ, V. Santana, Brno/CZ, A. Sojka, Brno/CZ, A. Marko, Brno/CZ, O. Martyniuk, Brno/CZ, J. Dubninska-Midlikova, Brno/CZ, A. Solodovnyk, Brno/CZ
- 09.30 a.m **Dynamical properties of electrolytes – insight from NMR relaxometry**
D. Kruk, Olsztyn/PL

10.00 a.m Coffee Break & Exhibition

Awards

Chair: J. Liermann

Audimax

- 10.30 a.m **Ernst Award** - M. Brammerloh
- 10.50 a.m **Ernst Award** - D. Joseph
- 11.10 a.m **Ernst Award** - M. Rudolph
- 11.30 a.m **Albert Overhauser Award** - A. Kuzhelev

12.00 p.m Lunch Break

Parallel 1A: Dynamic Nuclear Polarization

Chair: A. Kuzhelev

Audimax

- 01.30 p.m **Crystallization in confinement studied by solid-state NMR and MAS DNP**
G. Mollica, Marseille/FR, M. Juramy, Marseille/FR, S. Viel, Marseille/FR, F. Ziarelli, Marseille/FR, S. F. Cousin, Marseille/FR, P. Thureau, Marseille/FR
- 01.55 p.m **Bullet DNP With a Stripline Flow Probe**
K. Kouril, Karlsruhe/DE, K. Safiullin, Karlsruhe/DE, M. Minaei, Karlsruhe/DE, P. Singh, Karlsruhe/DE, M. Harder, Nijmegen/NL, H. Janssen, Nijmegen/NL, A. P. M. Kentgens, Nijmegen/NL, B. Meier, Karlsruhe/DE

Scientific Programme

- 02.15 p.m **Adiabatic DNP with Shaped Chirp Pulses**
S. A. Jegadeesan, Konstanz/DE, Y. Zhao, St Andrews/GB, H. El Mkami,
St Andrews/GB, R. Hunter, St Andrews/GB, G. Smith, St Andrews/GB,
I. Kuprov, Southampton/GB, G. Mathies, Konstanz/DE
- 02.35 p.m **On the Interplay of pulsed DNP and EPR**
N. Wili, Aarhus/DK, A. B. Nielsen, Aarhus/DK, J. P. Carvalho, Aarhus/DK,
N. Chr. Nielsen, Aarhus/DK

Parallel 1B: Dynamics & Relaxation

Chair: [U. Scheler](#)

[Arno-Esch-Lecture Hall 1](#)

- 01.30 p.m **Investigating structural protein dynamics by NMR spectroscopy at high magnetic fields**
N. A. Lakomek, Düsseldorf/DE
- 01.55 p.m **Global slow motions in biosolids studied by ^2H stimulated echo NMR**
A. Krushelnitsky, Halle/DE, F. Shahsavan, Halle/DE, G. Hempel,
Halle/DE, N. Fatkullin, Halle/DE
- 02.15 p.m **Effect of resins on SBR Dynamics by solid state NMR and NMR relaxometry**
M. Pierigé, Pisa/IT, F. Nardelli, Pisa/IT, L. Calucci, Pisa/IT, F. Martini,
Pisa/IT, M. Geppi, Pisa/IT, L. Giannini, Milan/IT, A. Causa, Milan/IT,
M. Cettolin, Milan/IT, E. R. deAzevedo, São Carlos/BR
- 02.35 p.m **Skin, fat, and spaghetti: investigations of co-existing solid and liquid phases in organic materials using solid-state NMR with dynamics-based spectral editing**
D. Topgaard, Lund/SE

Parallel 1C: Imaging & Diffusion

Chair: [M. Bruschewski](#)

[Arno-Esch-Lecture Hall 2](#)

- 01.30 p.m **Insights into Chemical Reactors at Industrial Conditions with Magnetic Resonance**
A. Sederman, Cambridge/GB
- 01.55 p.m **Advancing Electrophoretic NMR with Reference Electrodes**
S. Buyting, Münster/DE, M. Schönhoff, Münster/DE
- 02.15 p.m **Deuterated Nano-Polymers for Renal and Lymphatic Imaging via Quantitative Deuterium MRI**
L. M. Fries, Göttingen/DE, E. Montrazi, Rehovot/IL, H. Allouche-Arnon,
Rehovot/IL, A. Bar-Shir, Rehovot/IL, L. Frydman, Rehovot/IL, S. Glöggler,
Göttingen/DE
- 02.35 p.m **Metabolic magnetic resonance**
J.-B. Hövener, Kiel/DE

Scientific Programme

03.00 p.m. Poster Session 1 (odd numbers) & Coffee Break

Plenary Session

Chair: H. Oschkinat

Audimax

05.00 p.m. **Expanding the Tool Box for Structural Biology: ^{19}F MAS NMR with and without DNP for Protein Assemblies and Proteins in Cellular Environments**
T. Polenova, Newark/US, M. Akke, Stockholm/SE, D. Banks, Billerica/US, J. Kempf, Billerica/US, A. M. Gronenborn, Pittsburgh/US, M. Wang, Newark/US, C. M. Quinn, Newark/US, R. Zadorozhnyi, Newark/US, B. Runge, Newark/US, K. Tekwani Movellan, Newark/US, R. Kalabekova, Newark/US, W. Zhu, Pittsburgh/US, I. V. Sergeyev, Billerica/US, J. Struppe, Billerica/US

05.30 p.m. **Novel approaches for screening large sets of ligands**
J. G. Korvink, Karlsruhe/DE, N. MacKinnon, Karlsruhe/DE, M. Jouda, Karlsruhe/DE

06.00 p.m. **FGMR General Member's Assembly**

Audimax

08.00 p.m. **City Tours**



Magnetic resonance equipment, service, training & more

Complete systems including installation and user training

- 🔧 **Complete 300-800 MHz Varian VNMRs systems:** Shielded Oxford or Varian magnet, DB, ID or OneNMR NMR probe, Auto-tuning, 2-4 channels, latest OpenVnmrJ, Linux computer
- 🔧 **Bruker & Varian console upgrades:**
 - Old Bruker (AV DRX, AV1, Win XP or old Linux) console to AV2 (latest Linux or Windows)
 - Old Varian Mercury/Inova to VNMRs (latest OpenVnmrJ software, new Centos/Ubuntu)

NMR parts

- 🔧 **Magnets:** Oxford, Bruker, Magnex/Varian 300...800 MHz narrow & wide-bore, vertical or horizontal shielded/unshielded, incl. installation
- 🔧 **Probes:** Diverse Varian & Bruker 200...800 MHz liquids (DB, ID, OneNMR) and solids probes
- 🔧 **Spare parts:** boards, preamps, amplifiers... (Varian/Bruker)
- 🔧 **Upgrades:** autosamplers, probes, VT accessories (coolers), auto-tuning, gradients, solids...

Repairs / Services / Consulting

- 🔧 **NMR services (all vendors):** Repair of consoles, probes, amplifiers, hard/software upgrades
- 🔧 **Magnet services:** system relocation, quench recovery, vacuum pumping (all manufacturers)
- 🔧 **NMR consulting:** pulse sequences, courses ( Mnova , VnmrJ, general NMR)
- 🔧 **Representing:**  Mnova software,  STELAR Fast Field Cycling,  Barthel RF Amplifiers

We are always searching for NMR systems and parts!

Scientific Programme

Wednesday, September 11, 2024

Pleenary Session

Chair: N. C. Nielsen

Audimax

- 08.30 a.m **NMR Chemical Shifts Beyond Numbers: Understanding Electronic Structures and Coordination Environments**
Christophe Coperet, Zurich/CH
- 09.00 a.m **Electron Paramagnetic Resonance on a Chip for Operando Materials Research**
K. Lips, Berlin/DE, S. Künstner, Berlin/DE, M. Segantini, Berlin/DE, J. McPeak, Berlin/DE, K. P. Dinse, Berlin/DE, B. Naydenov, Berlin/DE, A. Chu, Stuttgart/DE, M. Kern, Stuttgart/DE, J. Anders, Stuttgart/DE, P. Fischer, Pfinztal/DE
- 09.30 a.m **Clinical Translation of Hyperpolarized MR**
J. Ardenkjær-Larsen, Kgs Lyngby/DK

10.00 a.m Coffee Break & Exhibition

Parallel 2A EPR

Chair: O. Schiemann

Audimax

- 10.30 a.m **Exploring the conformational landscape of membrane proteins using SDSL-EPR spectroscopy and computational modelling**
M. Elgeti, Leipzig/DE
- 10.55 a.m **Pulsed EPR methods in the angstrom to nanometre scale shed light on the conformational flexibility of a fluoride riboswitch**
L. Rimmel, Göttingen/DE, A. Meyer, Göttingen/DE, K. Ackermann, St Andrews/GB, G. Hagelueken, Bonn/DE, M. Bennati, Göttingen/DE, B. E. Bode, St Andrews/GB
- 11.15 a.m **Thin layer investigations of molecular qubits**
J. van Slageren, Stuttgart/DE, L. Tesi, Stuttgart/DE, R. Kataria, Stuttgart/DE, A. Allgaier, Stuttgart/DE, F. Stemmler, Stuttgart/DE, M. Kern, Stuttgart/DE
- 11.35 a.m **Fatty Acid Binding to Human Fatty Acid Binding Proteins (FABP) as Seen from a Ligand's Perspective**
D. Hinderberger, Halle (Saale)/DE, F. A. Schöffmann, Halle/DE, S. Michler, Halle/DE, D. Robaa, Halle/DE, J. Volmer, Halle/DE

Scientific Programme

Parallel 2B: Small Molecules & Applications

Chair: D. Michalik

Arno-Esch-Lecture Hall 1

- 10.30 a.m **NMR in targeted and non-targeted food analysis – from research to standardisation**
J. Teipel, Karlsruhe/DE, T. Kuballa, Karlsruhe/DE
- 10.55 a.m **Product Monitoring and Mechanism Research of PET Enzymatic Degradation with Liquid & Solid State NMR**
Z. Zhao, Leipzig/DE, A. Useini, Leipzig/DE, A. Zlobin, Leipzig/DE, P. Falkenstein, Leipzig/DE, E. Butenschön, Leipzig/DE, N. Bashirova, Leipzig/DE, J. Mao, Frankfurt/DE, W. Zimmermann, Leipzig/DE, G. Künze, Leipzig/DE, N. Sträter, Leipzig/DE, J. Matysik, Leipzig/DE, C. Sonnendecker, Leipzig/DE, C. Song, Leipzig/DE
- 11.15 a.m **High-pressure low-field NMR spectroscopy: New concepts and applications**
J. Denninger, Aachen/DE, S. A. Ortiz Restrepo, Aachen/DE, A. Duchowny, Aachen/DE, K. Linssen, Aachen/DE, A. Adams, Aachen/DE
- 11.35 a.m **Potentials and Applications of Solid-State NMR Spectroscopy in Organic Mechanochemistry**
T. Wiegand, Aachen/DE

Parallel 2C: Hyperpolarization

Chair: P. Schmieder

Arno-Esch-Lecture Hall 2

- 10.30 a.m **Quantitative ^1H and ^{13}C NMR Spectroscopy with Overhauser Dynamic Nuclear Polarization**
K. Münnemann, Kaiserslautern/DE, J. Phuong, Kaiserslautern/DE, S. Mross, Kaiserslautern/DE, H. Hasse, Kaiserslautern/DE
- 10.55 a.m **Nuclear Spin Hyperpolarization Through Metal-Free Activation of Parahydrogen (MF-PHIP)**
V. V. Zhivonitko, Oulu/FI, D. O. Zakharov, Oulu/FI, K. Konsewicz, Oulu/FI, K. Chernichenko, Helsinki/FI, K. Sorochkina, Helsinki/FI, J. Bresien, Rostock/DE, V.-V. Telkki, Oulu/FI, I. Pápai, Budapest/HU, A. Schulz, Rostock/DE, T. Repo, Helsinki/FI
- 11.15 a.m **Hyperpolarization of ^{15}N -pyridinium by using pH2 enables access to reactive oxygen sensors and pilot in vivo studies**
R. Mei, Göttingen/DE, L. Fries, Göttingen/DE, T. L. K. Hune, Göttingen/DE, M. D. Santi, Göttingen/DE, G. G. Rodriguez, Göttingen/DE, S. Sternkopf, Göttingen/DE, S. Glöggler, Göttingen/DE
- 11.35 a.m **Hyperpolarized ^{129}Xe in high-field and benchtop NMR**
L. Mitschang, Berlin/DE

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12.00 p.m Lunch Break

Scientific Programme

Magritek Lunch Workshop

12.00 p.m – 1:00 p.m

SR 126 (Building 1)

Parallel 3A: Interactions, Cells & Organisms

Chair: H. Heise

Audimax

- 01.30 p.m **Challenging the Limits of Characterising Weak Interactions in Dilute Solutions**
M. Erdelyi, Uppsala/SE
- 01.55 p.m **Characterization of Intact Fungal Cell-Wall Architecture Using Proton Detected Solid-State NMR Spectroscopy at 60-150 kHz MAS**
A. Lends, Riga/LV, M. Org-Tago, Tallin/EE, A. Kaldma, Tallin/LV, A. Samoson, Tallin/EE
- 02.15 p.m **Detecting protein hot-spot in live cells with high-performance ¹⁹F-tags**
X. C. Su, Tianjin/CN, C. Y. Cui, Tianjin/CN, B. Li, Tianjin/CN, Y. H. Xiao, Tianjin/CN
- 02.35 p.m **EPR Oxygen Imaging in Preclinical Tumors**
M. Elas, Kraków/PL, A. Drzał, Kraków/PL, A. Murzyn, Kraków/PL, G. Dziurman, Kraków/PL, A. Bienia, Kraków/PL, D. Szczygieł, Kraków/PL, B. Płóciennik, Kraków/PL, M. Szczygieł, Kraków/PL, M. Krzykawska-Serda, Kraków/PL

Parallel 3B: Solids & Materials

Chair: K. Seidel

Arno-Esch-Lecture Hall 1

- 01.30 p.m **From mass transport to atomic resolution on production of bio-based carbon fibers using MRI and NMR**
D. Bernin, Gothenburg/SE
- 01.55 p.m **Correlations between NMR-detected Polymer Chain Motion and Mechanical Properties of Biodegradable Semicrystalline Polyesters**
K. Saalwächter, Halle (Saale)/DE, A. Anuar, Halle (Saale)/DE, Q. Yu, Halle (Saale)/DE, T. Thurn-Albrecht, Halle (Saale)/DE
- 02.15 p.m **An Atomistic View on the Mechanism of Diatom Peptide-guided Biomimetic Silica Formation**
D. Kurzbach, Vienna/AT
- 02.35 p.m **Applications of Solid-State NMR Spectroscopy in Developments of Portland Cement Binders with Low CO₂ Footprint**
J. Skibsted, Aarhus/DK

Scientific Programme

Parallel 3C: Instrumentation & Methods

Chair: J. Schmedt auf der Günne

Arno-Esch-Lecture Hall 2

- 01.30 p.m **Old and new tricks for resonance assignment of large deuterated proteins with ^1H detection under fast MAS**
J. Stanek, Warsaw/PL, P. Paluch, Warsaw/PL, E. Kuc, Warsaw/PL, Z. Toleikis, Riga/LV, M.-L. Org-Tago, Tallin/EE, K. Vanatalu, Tallin/EE, A. Kaldma, Tallin/EE, R. Augustyniak, Warsaw/PL, A. Samoson, Tallin/EE, A. Lends, Riga/LV
- 01.55 p.m **Higher Fields, Smaller Coils, Spherical Spinning: High-Temperature Superconductor and a Tubular Insert for MAS NMR**
N. Alaniva, Zürich/CH, A. B. Barnes, Zürich/CH, C. Gao, Zürich/CH, P.-H. Chen, Zürich/CH, S. Björgvinsdottir, Zürich/CH, H. Birbaum, Zürich/CH, E. P. Saliba, Zürich/CH, J. H. J. Ellison, Zürich/CH, A. Däpp, Zürich/CH, R. Gunzenhauser, Zürich/CH, M. Urban, Zürich/CH, I. Gr. Pagonakis, Zürich/CH
- 02.15 p.m **Operando detection of dissolved oxygen in fluid solution using a submersible rapid scan EPR-on-a-chip (RS-EPRoC) dipstick sensor**
J. E. McPeak, Copenhagen/DK, M. Segantini, Berlin/DE, G. Marcozzi, Berlin/DE, I. Dona, Berlin/DE, S. Künstner, Berlin/DE, A. Chu, Stuttgart/DE, M. Kern, Stuttgart/DE, M. Poncelet, Morgantown/US, B. Driesschaert, Morgantown/US, J. Anders, Stuttgart/DE, K. Lips, Berlin/DE
- 02.35 p.m **^1H - ^{19}F CPMAS DNP NMR Investigation of Pharmaceutical Formulations**
A. C. Pinon, Gothenburg/SE, M. Šoltéssová, Gothenburg/SE, F. Aussenac, Gothenburg/SE, J. Schlagnitweit, Gothenburg/SE, C. Reiter, Gothenburg/SE, A. Porea, Gothenburg/SE, R. Melzi, Gothenburg/SE, F. Engelke, Gothenburg/SE, D. Martin, Gothenburg/SE, A. S. Ankarberg, Gothenburg/SE, L. Emsley, Gothenburg/SE, S. Schantz, Gothenburg/SE

03.00 p.m Poster Session 2 (even numbers) - Coffee Break & Exhibition

Roundtable Discussion AI in Magnetic Resonance

Chair: C. Griesinger

Audimax

- 05.00 p.m **Artificial Intelligence in Magnetic Resonance - Advances, Opportunities, and Challenges**
D. F. Hansen, London/UK, I. Kuprov, Southampton/UK, V. Orekhov, Gothenburg/SE, M. S. Vinding, Aarhus/DK

Young Scientists Programm

Audimax

- 06.00 p.m **Young Scientists Programm**

Scientific Programme

Thursday, September 12, 2024

Plenary Session

Chair: W. Kozminski

Audimax

- 08.30 a.m **NMR and MRI off the Beaten Track**
P. Galvosas, Wellington/NZ, D. A. Clarke, Wellington/NZ, E. H. Novotny, Rio de Janeiro/BR, J. Wang, Cambridge (MA)/US, S. Haber-Pohlmeier, Stuttgart/DE, M. Mehdizad, Wellington/NZ, D. J. Holland, Christchurch/NZ
- 09.00 a.m **Shining light on polyaspartates: Novel photoresponsive alignment media for structure elucidation**
C. M. Thiele, Darmstadt/DE, R. Hossain, Darmstadt/DE
- 09.30 a.m **Magnetic resonance one spin at a time**
J. Wrachtrup, Stuttgart/DE

10.00 a.m Coffee Break & Exhibition

Parallel 4A: Batteries & Catalysis

Chair: M. Schönhoff

Audimax

- 10.30 a.m **Solid-State NMR: A Spectroscopic Window into the Molecular World of Battery Materials?**
M. R. Hansen, Münster/DE
- 10.55 a.m **Solid-State NMR as a Toolbox Towards a Full Mechanistic Understanding of Catalytic Butene Dimerization**
M. Schröder, Rostock/DE, T. H. Vuong, Rostock/DE, M. Sardo, Aveiro/PT, I Marin Montesinos, Aveiro/PT, J. Rabeah, Rostock/DE, L. Mafra, Aveiro/PT, A. Brückner, Rostock/DE, B. Corzilius, Rostock/DE
- 11.15 a.m **Resolving Structures of Paramagnetic Systems in Chemistry and Materials Science by Solid-State NMR: the Revolving Power of Ultra-Fast MAS**
J. Koppe, Lyon/FR, A. J. Pell, Lyon/FR, K. J. Sanders, Lyon/FR, T. C. Robinson, Lyon/FR, A. L. Lejeune, Lyon/FR, D. Proriol, Solaize/FR, S. Wegner, Ettlingen/DE, A. Porea, Ettlingen/DE, F. Engelke, Ettlingen/DE, R. J. Clément, Santa Barbara/US, C. P. Grey, Cambridge/GB, G. Pintacuda, Lyon/FR
- 11.35 a.m **Magnetic resonance as a tool to investigate organic radical batteries**
J. Granwehr, Jülich/DE, D. T. Daniel, Jülich/DE

Scientific Programme

Parallel 4B: Quantum Sensing

Chair: F. Reinhard

Arno-Esch-Lecture Hall 1

- 10.30 a.m **Quantum Sensing: Materials Through Application**
D. Braje, Lexington/US
- 10.55 a.m **Harnessing Spin Defects in 2D Materials as Ultrathin Platforms for Nanoscale Magnetic Resonance**
R. Rizzato, Muenchen/DE, M. Helm, Dresden/DE, A. V. Stier, Muenchen/DE, J. J. Finley, Muenchen/DE, D. B. Bucher, Muenchen/DE, M. Schalk, Muenchen/DE, S. Mohr, Muenchen/DE, J. C. Hermann, Muenchen/DE, J. P. Leibold, Muenchen/DE, F. Bruckmaier, Muenchen/DE, G. Salvitti, Muenchen/DE, C. Qian, Muenchen/DE, J. Peirui, Muenchen/DE, G. Astakhov, Dresden/DE, U. Kentsch, Dresden/DE
- 11.15 a.m **Unraveling Loss Mechanisms in Microresonators for Electron Spin Detection in Sub-Nanoliter Volumes**
N. Abhyankar, College Park/US, M. Trusheim, Maryland/US, D. Fahey, Maryland/US, S. Blakley, Maryland/US
- 11.35 a.m **Towards in vivo single-molecule magnetic resonance spectroscopy with a diamond sensor**
F. Shi, Hefei/CN

Parallel 4C: Computation & Software

Chair: D. Paschek

Arno-Esch-Lecture Hall 2

- 10.30 a.m **New experimental and computational tools for mixture analysis - spectral "pseudo-dimensions" and Wasserstein metric**
K. Kazimierczuk, Warsaw/PL, A. Gambin, Warsaw/PL, B. Domżał, Warsaw/PL, B. Miasojedow, Warsaw/PL, P. Putko, Warsaw/PL, J. Romero, Warsaw/PL, E. Nawrocka, Warsaw/PL, D. Gołowicz, Warsaw/PL
- 10.55 a.m **Using Neural Networks for Analyzing NMR Time Series**
J. Hellwig, Rostock/DE, K. Neymeyr, Rostock/DE
- 11.15 a.m **Optimal Control Strategies for Pulsed Dynamic Nuclear Polarization Sequence Design**
J. P. Carvalho, Aarhus/DK, D. L. Goodwin, Aarhus/DK, N. Wili, Aarhus/DK, A. B. Nielsen, Aarhus/DK, N. C. Nielsen, Aarhus/DK
- 11.35 a.m **www.nmrium.org: Revolutionizing NMR spectra processing with a web-based application**
L. Patiny, Lonay/CH, A. Bolaños, Lonay/CH, M. Zasso, Lonay/CH, H. Musallam, Jena/DE

Scientific Programme

12.00 p.m Lunch Break

Parallel 5A: Biological Systems

Chair: B. Joseph

Audimax

- 01.30 p.m **Following conformational changes in LbuCas13a from apo to the ternary cr- and target RNA bound state with EPR spectroscopic distance measurements**
M. F. Vicino, Bonn/DE, C. Allar, Bonn/DE, O. Schiemann, Bonn/DE
- 01.55 p.m **Amino-acid Side Chains as conformational reporters of PI3K-SH3 unfolding studied by DNP-Enhanced ssNMR**
L. Levorin, Jülich/DE, L. Gardon, Jülich/DE, M. Jaspert, Jülich/DE, N. Rüter, Jülich/DE, P. Neudecker, Jülich/DE, H. Heise, Jülich/DE
- 02.15 p.m **Study on the extracellular loops of the Outer membrane protein G in native membrane environment**
M. Adélaïde, Berlin/DE, F. Lindemann, Berlin/DE, M. Abbas, Berlin/DE, M. Herrera Glomm, Berlin/DE, E. P. Saliba, Zurich/CH, N. Cremer, Berlin/DE, A.B. Barnes, Zurich/CH, H. Oschkinat, Berlin/DE
- 02.35 p.m **The many hurdles on the way to investigating PTEN with NMR, and how to overcome them**
T. Viennet, Aarhus/DK, D. R. Dempsey, Boston/US, R. Iwase, Boston/US, P. A. Cole, Boston/US, H. Arthanari, Boston/US

Parallel 5B: Structure & Crystallography

Chair: H. Kogler

Arno-Esch-Lecture Hall 1

- 01.30 p.m **MAS NMR of amorphous calcium carbonate provides proof for the pre-nucleation cluster pathway**
G. Mathies, Konstanz/DE, M. Gindele, Hannover/DE, S. Vinod-Kumar, Konstanz/DE, V. S. Redrouthu, Konstanz/DE, D. Gebauer, Hannover/DE
- 01.55 p.m **Ionic Liquid Films in Porous Media - Insight from Solid-state NMR Spectroscopy**
D. Wisser, Erlangen/DE, C. L. Tavera-Méndez, Erlangen/DE, A. Bergen, Erlangen/DE, M. Frosch, Erlangen/DE, P. Agüero, Erlangen/DE, S. Trzeciak, Erlangen/DE, D. Zahn, Erlangen/DE, K. Meyer, Erlangen/DE, M. Hartmann, Erlangen/DE
- 02.15 p.m **¹¹B Quadrupole / ¹¹B-¹⁹F Dipole-Dipole Interference in BODIPY-type Molecules**
M. John, Göttingen/DE, D. Franke, Göttingen/DE, X. Wang, Göttingen/DE, D. Stalke, Göttingen/DE, F. Rüttger, Göttingen/DE
- 02.35 p.m **Secret life of molecular crystals: a solid-state NMR perspective**
M. Dudek, Łódź/PL, P. Paluch, Łódź/PL, P. Nowak, Łódź/PL, D. Senthurpandi, Łódź/PL, A. Jeziorna, Łódź/PL

Scientific Programme

Parallel 5C: In-Situ & Operando

Chair: W. Baumann

Arno-Esch-Lecture Hall 2

- 01.30 p.m **Investigations of Heterogeneously Catalysed Gas-Liquid Reactions under Industrially Relevant Conditions with Benchtop NMR Spectroscopy**
E. v. Harbou, Kaiserslautern/DE, P. Sterner, Kaiserslautern/DE, D. Holland, Christchurch/NZ, O. Bey, Ludwigshafen/DE, V. Streitferdt, Ludwigshafen/DE, R. Berg, Ludwigshafen/DE, E. Steimers, Ludwigshafen/DE
- 01.55 p.m **Operando electron paramagnetic resonance spectroscopy for elucidating the behavior of paramagnetic catalytic sites during low-temperature NH₃-SCR of NO**
T. H. Vuong, Rostock/DE, T. Doan, Hanoi/VN, M. T. Le, Hanoi/VN, T. H. Pham, Hanoi/VN, J. Rabeah, Rostock/DE, A. Brückner, Rostock/DE
- 02.15 p.m **Time-Resolved Diffusion NMR a tool for reaction monitoring and beyond**
M. Urbańczyk, Warszawa/PL
- 02.35 p.m **In-situ and operando Electron Paramagnetic Resonance applied for investigation of copper zeolite based catalysts**
S. Mossin, Lyngby/DK, Q. Gao, Lyngby/DK

03.00 p.m Coffee Break

Awards

Chair: J. Matysik

Audimax

- 03.30 p.m **Lifetime Membership**.- T. Prisner
Otto Stern Award - H. Kessler
Poster Awards & Closing - B. Corzilius

Editorial Insights - Wiley (Weinheim)

Arno-Esch-Lecture Hall 1

- 05.30 p.m **Working in Scientific Publishing** - A. Straube

06.00 p.m Depature for Conference Dinner

Conference Dinner

- 07.00 p.m **Conference Dinner** -Tiergartenalle 6, Trotzenburg