

The International Bologna Conference on Magnetic Resonance in Porous Media, acronym MRPM, was first started at the University of Bologna, Italy, in 1990. In the past thirty years, MRPM travels across the world from Italyto UK, Belgium, Norway, Germany, France, USA, New Zealand. Over the years, MRPM becomes a gathering point for scholars, students and industrial professionals to exchange ideas and collaborate on important projects. It develops an inclusive culture for different people and diverse topics.

This year, the 15th MRPM conference travels to China, and to the beautiful city of Hangzhou. Hangzhou locates in the Zhejiang Province of China, one hundred kilometers south of Shanghai. Hangzhou was once the capital city of China about one thousand years ago. It was the east end of the silk road as it has been producing world-famous silk and tea for more than a thousand years. It is called "the heaven" in China for its gorgeous view of West Lake and the quiet retreats in tea plantation hills. Nowadays, Hangzhou is an economic powerhouse thanks to the fast development of internet economy.

MRPM15 is hosted by Zhejiang University, a prestigious multidisciplinary higher-education institute in China. It constitutes seven campuses and hosts more than 60,000 students. The people in Zhejiang University participate in top-level academic and industrial research activities. The university has a solid-state NMR center and a medical magnetic resonance imaging center. It also supports diverse research groups in the areas related to porous media.

The honorary chairman of this conference is Professor Jiangfeng Du who is known for the pioneering work in single molecular detection by magnetic resonance. The executive chairmen of the conference are Professor Xueqian Kong and Professor Ruiliang Bai.



# CONFERENCE COMMITTEE

### **CONFERENCE CHAIRS**

Honorary Chair 2022: Jiangfeng Du Conference Chair 2022: Xueqian Kong Ruiliang Bai

### **Local Organizing Committee:**

Lizhi Xiao Zhong Chen Feng Deng Fazhan Shi Wei Wang Dan Wu Xin Zhou

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Chair: Yi-Qiao Song

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Treasurer: Siegfried Stapf

# KEYNOTE + INVITED SPEAKERS

### **Keynote Speakers**

Jeffrey A. Reimer, University of California, Berkeley, USA

Peter J. Basser, NIH, USA

Leonardo Brizi, University of Bologna, Italy

Klaus Schmidt-Rohr, Brandeis University, USA

Jiangfeng Du, University of Science and technology of China, China

Lizhi Xiao, China University of Petroleum, China

Xin Zhou, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, China

Zhong Chen, Xiamen University, China

Wei Wang, Lanzhou University, China

### **Invited speakers**

Rustem Valiullin, Leipzig University, Germany

Christoph H. Arns, University of New South Wales, Australia

Alexej Jerschow, New York University, USA

Aaron J. Rossini, Iowa State University, USA

Tito José Bonagamba, University of São Paulo, Brasil

Ville-Veikko Telkki, University of Oulu, Finland

Evren Ozarslan, Linköping University, Sweden

William S. Price, Western Sydney University, Australia

Sharon E. Ashbrook, University of St Andrews, UK

Yongchao Su, Merck, USA

Dimitrios Sakellariou, KU Leuven, Belgium

Villiam Bortolotti, University of Bologna, Italy

Ileana O Jelescu, Lausanne University Hospital (CHUV) and University of Lausanne (UNIL),

Switzerland

Magnus Herberthson, Linköping University, Sweden

Yue Wu, University of North Carolina at Chapel Hill, USA

Kong Ooi Tan, École Normale Supérieure, France

Gerd Buntkowsky, TU Darmstadt, Germany

Yefeng Yao, East China Normal University, China

Hua Guo, Tsinghua University, China

Dan Wu, Zhejiang University, China
Chunsheng Zhou, Harbin Institute of Technology, China
Zheng Xu, Chongqing University, China
Fangrong Zong, Beijing University of Posts and Telecommunications, China
Jun Xu, Wuhan Institute of Physics and Mathe-matics, Chinese Academy of Sciences, China
Guangjin Hou, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China
Luming Peng, Nanjing University, China
Bingwen Hu, East China Normal University, China

# NMR SCHOOL SPEAKERS

Yiqiao Song, Harvard University, USA
Bernhard Blümich, RWTH Aachen University, Germany
Daniel Topgaard, Lund University, Sweden
Ben Newling, University of New Brunswick, Canada
Zonghai Harry Xie, CoreLab, USA
Bruce J. Balcom, University of New Brunswick, Canada

# **Local Organizing Institute**

**Department of Chemistry Zhejiang University** 

http://www.chem.zju.edu.cn/

Zhejiang University Interdisciplinary Institute of Neuroscience and Technology

http://www.ziint.zju.edu.cn/

**MOE Frontier Science Center for Brain Science and Brain-Machine Integration** 

http://www.neuroscience.zju.edu.cn/

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# Program-AT-A-Glance

| NMR SCHOOL, ZO                 |                    | Beijing 20:00-24:00, New York 8:00-12:00, Berlin 14:00-18:00)       |
|--------------------------------|--------------------|---|
| SUNDAY,                        | 19:55-20:00        | Opening Speech  |
| AUGUST 21 <sup>ST</sup> 2022   | 20:00-24:00        | Tutorial Lectures   |
| MRPM15, ZOOM (                 | Aug 22 to Aug 2    | 24, Beijing 20:00-24:00, New York 8:00-12:00, Berlin 14:00-18:00)   |
|                                | 20:00-20:15        | Welcome Remarks   |
| MONDAY,                        | 20:15-22:00        | Keynote Session 1 (Jeffery A. Reimer & Peter J. Basser)             |
| AUGUST 22 <sup>ND</sup> , 2022 | 22.00 24.00        | Session 1: Methodology and Geophysics                               |
| 22 , 2022                      | 22:00-24:00        | Session 2: Hardware development and applications                    |
|                                | 20:00-20:45        | Keynote Session 2 (Leonardo Brizi)                                  |
| TUESDAY,                       | 20.45.22.00        | Session 3: Low field MR and Applications                            |
| AUGUST                         | 20:45-22:00        | Session 4: Relaxometry and Dynamics                                 |
| 23 <sup>RD</sup> , 2022        | 22.10.24.00        | Session 5: Diffusion and Dynamics                                   |
|                                | 22:10-24:00        | Session 6: New Applications of MR                                   |
|                                | 20:00-20:45        | Keynote Session 3 (Klaus Schmidt-Rohr)                              |
| WEDNESDAY,                     | 20 45 22 00        | Session 7: Solid-state and Nanoporous Materials                     |
| AUGUST                         | 20:45-22:00        | Session 8: Relaxometry and related topics                           |
| 24 <sup>TH</sup> , 2022        | 22 10 24 00        | Session 9 - Biomedicine, Biophysics, and MRI                        |
|                                | 22:10-24:00        | Session 10 - Adsorption in Porous Materials                         |
| MRPM15, IN-PERS                | SON (Aug 25 to     | Aug 26, Beijing 8:30-18:00, New York 20:30-6:00, Berlin 2:30-12:00) |
| The attendees can atte         | end the conference | ce either online or in person.                                      |
|                                | 08:30-08:40        | Opening Speech  |
|                                | 08:40-10:10        | Keynote Session 4 (Jiangfeng Du & Lizhi Xiao)                       |
| THURCDAY                       | 10:10-10:30        | Photos & Coffee Break   |
| THURSDAY,<br>AUGUST            | 10:30-12:00        | Session 11  |
| 25 <sup>TH</sup> , 2022        | 12:00-13:30        | Lunch break   |
| ,                              | 13:30-15:05        | Session 12  |
|                                | 15:05-16:00        | Poster Session  |
|                                | 16:00-18:00        | Session 13  |
|                                | 08:30-10:30        | Session 14  |
|                                | 10:45-12:00        | Session 15  |
| FRIDAY,                        | 12:00-13:30        | Lunch break   |
| AUGUST                         | 13:30-15:05        | Session 16  |
| 26 <sup>TH</sup> , 2022        | 15:20-17:10        | Session 17  |
|                                | 17:10-18:00        | Awards & Closing ceremony   |
|                                |                    |   |



# NMR SCHOOL SCHEDULE

Beijing Time

# SUNDAY, AUGUST 21<sup>ST</sup> 2022 ZOOM ONLINE

# Chair: Xueqian Kong & Ruiliang Bai

| 19:55 – 20:00 | Opening speech   |
|---------------|--|
| 20:00 – 20:40 | Lecture 1: Yiqiao Song, Harvard University, USA, The history, current, and future of magnetic resonance in porous media                        |
| 20:40 – 21:20 | Lecture 2: Bernhard Blümich, RWTH Aachen University, Germany, NMR Hardware   |
| 21:20 – 22:00 | Lecture 3: Daniel Topgaard, Lund University, Sweden, <i>Translational motion and magnetic field gradients</i>                                  |
| 22:00 – 22:40 | Lecture 4: Ben Newling, University of New Brunswick, Canada, <i>Take</i> the current when it serves: flow quantification in magnetic resonance |
| 22:40 – 23:20 | Lecture 5: Zonghai Harry Xie, Core Lab, USA, NMR Applications in Rock Core Analysis – from Conventional to Unconventional                      |
| 23:20 – 24:00 | Lecture 6: Bruce J. Balcom, University of New Brunswick, Canada,  Magnetic Resonance Imaging of Materials                                      |

### **MRPM15 SCHEDULE**

## Beijing Time

# MONDAY, AUGUST 22<sup>ND</sup> 2022 ZOOM ONLINE

# **MRPM15** Conference Opening Ceremony

20:00 – 20:15 Welcome Remarks

### **Keynote Session 1**

Chair: Xueqian Kong & Ruiliang Bai

| 20:15 – 21:00 | Keynote lecture: Jeffrey A. Reimer, University of California,           |
|---------------|---|
|               | Berkeley, USA, A Molecular View of Carbon Capture with Porous Materials |
| 21:00 - 21:45 | Keynote lecture: Peter J. Basser, NIH, USA, Probing Tissue              |
|               | Microstructure and Function   |

### **Coffee Break**

21:45 - 22:00

### Session 1 - Methodology and Geophysics

Chair: Yiqiao Song, Harvard University, USA

| 22:00 – 22:25 | Invited lecture 1: Rustem Valiullin, Leipzig University, Germany,           |
|---------------|---|
|               | Advanced NMR cryoporometry  |
| 22:25 – 22:50 | Invited lecture 2: Christoph H. Arns, University of New South Wales,        |
|               | Australia, NMR response interpretation utilizing Digital Rock Physics       |
| 22:50 – 23:05 | Normal oral 1: Jing Li, University of Oulu, Finland, 129Xe NMR analysis     |
|               | reveals efficient gas transport between inborn micro-, meso- and macropores |
|               | in geopolymers  |
| 23:05 - 23:13 | Short oral 1: Alfredo Ordinola, Linköping University, Sweden,               |
|               | Measurement of the apparent diffusion propagator                            |
| 23:13 – 23:21 | Short oral 2: Sabine Kruschwitz, Bundesanstalt für Materialforschung        |
|               | und -prüfung (BAM) und TU Berlin, Germany, Non-destructive testing          |
|               | application examples using the NMR core-analyzing tomograph                 |
| 23:21 – 23:29 | Short oral 3: Tatiana Monaretto, Center National De La Recherche            |
|               | Scientifique (CNRS), France, Dynamics of pore filling by                    |
|               | spatially-resolved relaxometry  |
| 23:29 - 23:37 | Short oral 4: Siegfried Stapf, TU Ilmenau, Germany, Ageing of reservoir     |
|               | rocks: a multinuclear NMR relaxometry study                                 |
| 23:37 – 23:45 | Short oral 5: Mark Armstrong, University of Windsor, Canada,                |
|               | Optimized Phase Cycling for Coherence Pathway Selection in Unbalanced       |
|               | Fast Spin-Echo  |
| 23:45 - 23:53 | Short oral 6: Shin Utsuzawa, Schlumberger, USA, Ringing cancellation        |
|               | in Carr-Purcell-Meiboom-Gill-type sequences                                 |
|               |   |



### Session 2 – Hardware development and applications

Chair: Bernhard Blümich, RWTH Aachen University, Germany

| 22:00 – 22:25 | Invited lecture 1: Alexej Jerschow, New York University, USA, MRI        |
|---------------|--|
|               | and magnetometry techniques for battery research and development         |
| 22:25 – 22:50 | Invited lecture 2: Dimitrios Sakellariou, KU Leuven, Belgium,            |
|               | Custom-made Magnetic Resonance: An application-driven instrumentation    |
|               | approach for materials engineering                                       |
| 22:50 – 23:15 | Invited lecture 3: Kong Ooi Tan, École Normale Supérieure, Building      |
|               | a 263 GHz Pulsed DNP Microwave Bridge, Waveguides, Probe, and MAS        |
|               | Drive Caps   |
| 23:15 - 23:30 | Normal oral 1: Thomas Hiller, Federal Institute for Geosciences and      |
|               | Natural Resources (BGR), Germany, Towards a mobile soil moisture         |
|               | mapping application based on prepolarized surface-NMR                    |
| 23:30 - 23:45 | Normal oral 2: Shiwen Chen, RIPED Petrochina, China, Development         |
|               | and Applications of the MR Multi-Phase Flowmeter                         |
| 23:45 – 24:00 | Normal oral 3: Xiaoguang Zhao, Tsinghua University, China,               |
|               | Improving unilateral magnetic resonance efficiency using                 |
|               | metamaterial-enhanced radio frequency coil                               |
| 24:00 - 24:08 | Short oral 1: William Selby, University of New Brunswick, Canada, A      |
|               | Simple Portable Magnetic Resonance Technique for Characterizing Circular |
|               | Couette Flow of Non-Newtonian Fluids                                     |
|               |  |

# TUESDAY, AUGUST 23<sup>RD</sup> 2022 ONLINE

### **Keynote Session 2**

Chair: Sabina Haber-Pohlmeier, Universität Stuttgart, Germany

20:00 – 20:45 **Keynote lecture:** Leonardo Brizi, University of Bologna, Italy, *Recent* 

advances on single-sided NMR applications and proof of concept of low-field

NMR Fingerprinting aided by Artificial Intelligence

### Session 3 – Low field MR and Applications

Chair: Xiaoguang Zhao, Tsinghua University, China

| 20:45 – 21:10 | Invited lecture 1: Tito José Bonagamba, University of São Paulo,            |
|---------------|---|
|               | Brasil, NMR signals from mechanically oscillating samples in a single-sided |
|               | magnet: a simple Logging-While-Drilling simulator                           |
| 21:10 – 21:25 | Normal oral 1: Eric Schmid, Karlsruhe Institute of Technology,              |
|               | Germany, Low-Field NMR Sensor for Inline-Quality Control Applications       |
| 21:25 - 21:40 | Normal oral 2: Rui Chen, University of Shanghai for Science and             |
|               | Technology, China, Study on low-field nuclear magnetic resonance            |
|               | analytical technique of edible oil  |
| 21:40 – 21:48 | Short oral 1: Agide Gimenez Marassi, University of São Paulo, Brazil,       |
|               | NMR signals from oscillating samples in the presence of a magnetic field    |
|               | gradient  |
| 21:48 – 21:56 | Short oral 2: Henry R. N. B. Enninful, Leipzig University, Germany,         |
|               | Advanced Kernel-Based NMR Cryoporometry Characterization of                 |
|               | Mesoporous Solids   |

### Session 4 – Relaxometry and Dynamics

Chair: Siegfried Stapf, TU Ilmenau, Germany

| 20:45 – 21:10 | Invited lecture 1: Ville-Veikko Telkki, University of Oulu, Finland,           |
|---------------|--|
|               | Ultrafast multidimensional relaxation and diffusion measurements               |
| 21:10 – 21:25 | Normal oral 1: Manuel I. Velasco, Universidad Nacionla de Cordoba,             |
|               | Argentina, Organic matter detection in $T_1$ - $T_2$ relaxation maps for shale |
|               | reservoirs   |
| 21:25 – 21:40 | Normal oral 2: Mohammad Sadegh Zamiri, University of New                       |
|               | Brunswick, Canada, Shale Characterization Using 2D Magnetic Resonance          |
|               | $T_1$ - $T_2^*$ Relaxation Correlation and SPRITE MRI                          |
| 21:40 – 21:55 | Normal oral 3: Tristhal Parasram, University of Windsor, Canada,               |
|               | Magnetic Resonance $T_1$ Spectrum Analysis with Neural Networks                |

### Coffee Break

22:00 - 22:10



### Session 5 – Diffusion and Dynamics

Chair: Fangrong Zong, Beijing University of Posts and Telecommunications

| 22:10 – 22:35 | Invited lecture 1: Evren Özarslan, Linköping University, Sweden,             |
|---------------|--|
|               | Characterizing structural heterogeneity and water dynamics with novel        |
|               | diffusion MR   |
| 22:35 – 23:00 | Invited lecture 2: William S. Price, Western Sydney University,              |
|               | Australia, Faster NMR Diffusion Measurements for Porous Media and            |
|               | Reactions  |
| 23:00 - 23:15 | Normal oral 1: Benedict Newling, University of New Brunswick,                |
|               | Canada, Laminar Velocity Profile Measurements from Spin Echoes at            |
|               | Incomplete Polarization  |
| 23:15 - 23:23 | Short oral 1: Anne Selent, University of Oulu, Finland, Laplace NMR          |
|               | study of surfactants in aqueous solutions                                    |
| 23:23 – 23:31 | Short oral 2: Sarah Mailhiot, University of Oulu, Finland, 2D variable       |
|               | echo time CPMG acquisition for D- $T_2$ correlation measurements utilizing a |
|               | constant gradient  |
| 23:31 – 23:39 | Short oral 3: Alice Ducroix, Laboratoire PHENIX, Sorbonne                    |
|               | Université, CNRS, France, Dynamics and molecular transport of water          |
|               | inside boehmite suspensions probed by PFG-NMR                                |
| 23:39 – 23:47 | Short oral 4: Carlo Golini, University of Bologna, Italy, A single-sided     |
|               | NMR procedure to study structural differences of the cartilage tissue        |
| 23:47 – 23:55 | Short oral 5: Arthur Gustavo de Araujo -Ferreira, University of São          |
|               | Paulo, Brazil, A Benchtop Single-Sided RF-Shielded Magnet for Low Field      |
|               | NMR applications   |

### Session 6 – New Applications of MR

Chair: Zonghai Harry Xie, CoreLab, USA

| 22:10 - 22:35 | Invited lecture 1: Aaron J. Rossini, Iowa State University, USA,               |
|---------------|--|
|               | Structural Characterization of Boron Nitride and Oxide Materials by Dynamic    |
|               | Nuclear Polarization and Ultrahigh Field 35 T Solid-State NMR Spectroscopy     |
| 22:35 - 23:00 | Invited lecture 2: Yongchao Su, Merck, USA, Molecular Details of               |
|               | Amorphous Pharmaceuticals from Solid-State NMR and X-ray Atomic Pair           |
|               | Distribution Function  |
| 23:00 - 23:15 | Normal oral 1: Jyotsana Ojha, Indian Institte of Science Education and         |
|               | Research Mohali India, India, NMR spectroscopic approach to investigate        |
|               | the dynamics and heterostructure of fluorinated ionic liquids and their binary |
|               | mixtures   |
| 23:15 - 23:23 | Short oral 1: Siegfried Stapf, TU Ilmenau, Germany, Binary fluid               |
|               | systems in porous media: redistribution of miscible and immiscible fluids and  |
|               | the effect on their relaxation properties                                      |

| 23:23 – 23:31 | Short oral 2: Bulat Gizatullin, Technische Universität Ilmenau,          |
|---------------|--|
|               | Germany, Studying of Radicals on the Surface by DNP FFC: Ageing or       |
|               | Origin?  |
| 23:31 - 23:39 | Short oral 3: Tian He, Zhejiang University, China, Cortical Bone under   |
|               | Ultrahigh Magnetic Field: Relaxation, Spectroscopy and Micron-resolution |
|               | Imaging  |
| 23:39 - 23:47 | Short oral 4: Yashu Kharbanda, University of Oulu, Finland, Cheese       |
|               | Maturation Studies by Single-Sided Magnet                                |
| 23:47 – 23:55 | Short oral 5: Tiia Jacklin, University of Oulu, Finland, Modeling Xe     |
|               | NMR in carbon nanotubes  |
|               |  |



## WEDNESDAY, AUGUST 24<sup>TH</sup> 2022 ONLINE

### **Keynote Session 3**

Chair: Xueqian Kong, Zhejiang University, China

20:00 – 20:45 **Keynote lecture:** Klaus Schmidt-Rohr, Brandeis University, USA,

Solid-State NMR of Polymer–MOF Composites

20.45 – 20.50 Introducing MRPM16 (Kate Anderson)

### Session 7 - Solid-state and Nanoporous Materials

Chair: Ben Newling, University of New Brunswick, Canada

| 20:50 - 21:15 | Invited lecture 1: Sharon E. Ashbrook, University of St Andrews, UK,              |
|---------------|---|
|               | Exploiting <sup>17</sup> O Isotopic Enrichment in NMR Spectroscopy of Microporous |
|               | Materials   |
| 21:15 – 21:30 | Normal oral 1: Jun Xu, Nankai University, China, Deconvolution of                 |
|               | Metal Apportionment in Bulk Metal—Organic Frameworks                              |
| 21:30 – 21:45 | Normal oral 2: Frédérique Pourpoint, Centrale Lille, France, Solid-State          |
|               | NMR to study Metal-Organic Frameworks   |
| 21:45 – 22:53 | Short oral 1: Jeremias C. Zill, Leipzig University, Germany, Kinetics of          |
|               | a structural phase transition in MIL-53(Al)-NH <sub>2</sub>                       |
| 21:53 – 22:01 | Short oral 2: Daniil I. Kolokolov, Boreskov Institute of Catalysis,               |
|               | Russia, Probing light hydrocabons mobility by <sup>2</sup> H NMR in nanoporous    |
|               | UiO-66 MOF: effects of inorganic centers hydroxylation and framework              |
|               | defects   |

### $Session \ 8-Relaxometry \ and \ related \ topics \ \textbf{-}II$

Chair: Ruiliang Bai, Zhejiang University, China

| 20:50 – 21:15 | Invited lecture 1: Villiam Bortolotti, University of Bologna, Italy,        |
|---------------|---|
|               | Inversion problems and robust NMR parameter estimation: the Uniform         |
|               | Penalty principle extension Mupen   |
| 21:15 - 21:30 | Normal oral 1: Keelan T. O'Neill, University of Western Australia,          |
|               | Australia, Pore size and relaxation characterisation of Lunar and Martian   |
|               | planetary simulants   |
| 21:35 - 21:45 | Normal oral 2: Neil Robinson, University of Western Australia,              |
|               | Australia, Functional group resolved relaxation in porous media             |
| 21:45 – 21:53 | Short oral 1: Arthur Gustavo Araújo-Ferreira , University of Sao Paulo,     |
|               | Brazil, NMR on Porous Media: Surface relaxivity and Magnetic Susceptibility |
| 21:53 - 22:01 | Short oral 2: Can Liang, Changzhou Institute of Technology, China,          |
|               | Rock Wettability Characterization Using NMR Free Induction Decay            |
| Coffee Break  |   |
| 22:01 – 22:10 |   |



### Session 9 -Biomedicine, Biophysics, and MRI

Chair: Evren Ozarslan, Linköping University, Sweden

| 22:10 - 22:35 | Invited lecture 1: Ileana O Jelescu, Lausanne University Hospital                 |
|---------------|---|
|               | (CHUV) and University of Lausanne (UNIL), Switzerland, Water                      |
|               | exchange across cell membranes in brain gray matter                               |
| 22:35 - 23:00 | Invited lecture 2: Magnus Herberthson, Linköping University,                      |
|               | Sweden, The influence of diffusion across semi-permeable membranes on the         |
|               | MR signal: Insights from a one-dimensional model                                  |
| 23:00 – 23:15 | Normal oral 1: Ke Dai, Shanghai Jiao Tong University, China,                      |
|               | High-resolution diffusion-weighted MRI combining markerless prospective           |
|               | motion correction and locally low-rank constrained reconstruction                 |
| 23:15 – 23:30 | Normal oral 2: Jonathan L. MacNeil, University of Windsor, Canada,                |
|               | T <sub>2</sub> Mapping using Fast Spin Echo with Point Spread Function Correction |
| 23:30 – 23:45 | Normal oral 3: Yonghong Ding, Max Planck Institute for                            |
|               | Multidisciplinary Science, Germany, In-cell real-time monitoring of               |
|               | pyruvate metabolic conversion on Parkinson cell models via para-hydrogen          |
|               | induced polarization (PHIP)   |
| 23:45 – 23:53 | Short oral 1: Alfredo Ordinola, Linköping University, Sweden,                     |
|               | Characterizing structure and diffusion exchange: Comparing subsampling            |
|               | strategies  |
| 23:53 – 24:01 | Short oral 2: Yu Zeng, Zhejiang University, Comparisons of Parkinson's            |
|               | Disease Related Patterns in ASL MRI and FDG PET                                   |

# Session 10 – Adsorption in Porous Materials

Chair: Daniel Topgaard, Lund University, Sweden

| 22:10 – 22:35 | Invited lecture 1: Yue Wu, University of North Carolina at Chapel                      |
|---------------|--|
|               | Hill, USA, Correlations of Microscopic and Macroscopic Properties of                   |
|               | Porous Media Obtained by NMR-detected Isotherm Technique                               |
| 22:35 – 23:00 | Invited lecture 2: Gerd Buntkowsky, TU Darmstadt, Germany,                             |
|               | Solid-state NMR and DNP studies of guest molecules confined in porous silica materials |
| 23:00 – 23:15 | Normal oral 1: Chevallier-Boutell I J, IFEG, Argentina, Non-negligible                 |
|               | interactions of alkanes with silica mesopores affect self-diffusivity: a combined      |
|               | experimental and theoretical approach  |
| 23:15 – 23:30 | Normal oral 2: Janis Hessling, University of Münster, Germany, Spin                    |
|               | relaxation studies of an ionic liquid-based electrolyte confined in porous             |
|               | materials  |
| 23:30-23:45   | Normal oral 3: Minghui Zhang, Inner Mongolia Agricultural                              |
|               | University, China, Cell Wall Water States in Wood Studied by TDNMR                     |
|               | during Adsorption  |
|               |  |

|         |               |                                       | Manyahan makerika              |
|---------|---------------|---------------------------------------|--------------------------------|
| 23:45 – | 23:53 Short o | ral 1: Roya Khalili, University of Ou | ulu, Finland, Local structures |

| 23:45 - 23:53 | Short oral 1: Roya Khalili, University of Oulu, Finland, Local structures |
|---------------|---|
|               | and adsorption properties of rare earth phosphates                        |
| 23:53 - 24:01 | Short oral 2: Marie Bernardi, The University of Mons, Belgium,            |
|               | Benchtop NMR relaxometry for the follow-up of Ni(II) removal by three ion |
|               | exchange resins.  |



# THURSDAY, AUGUST 25<sup>TH</sup> 2022 (HYBRID)

金溪山庄,杭州市西湖区杨公堤 39号

08:30 – 08:40 am **Opening speech** 

### Chair: Zhou Xin, Wuhan Institute of Physics and Mathematics, China

08:40 – 09:25 am **Keynote lecture 1**: Jiangfeng Du, University of Science and

technology of China, China, Single molecule magnetic resonance

spectroscopy and imaging

09:25 – 10:10 am **Keynote lecture 2**: Lizhi Xiao, China University of Petroleum,

China, Borehole NMR Inside-out Imager for Porous Materials

### **Coffee Break and Photo**

10:10 - 10:30

### **Session 11**

### Chair: Wei Wang, Lanzhou University, China

| 10:30 – 10:55 am | Invited lecture 1: Yefeng Yao, East China Normal University, China,         |
|------------------|---|
|                  | Molecularly targeted MRI and MRS  |
| 10:55 – 11:10 am | Oral 1: Zhihao Long, China University of Petroleum (Beijing), China,        |
|                  | Determining Winding Patterns for RF Coils on Downhole Magnetic              |
|                  | Resonance Imaging Tool Using Stream Functions and Target-Field Method       |
| 11:10 – 11:25 am | Oral 2: J. Beau W. Webber, Lab-Tools Ltd., UK, The implementation of        |
|                  | an easy-to-apply NMR Cryoporometric instrument for porous materials         |
| 11:25 – 11:40 am | Oral 3: Xinyu Zhang, China University of Petroleum (Beijing), China,        |
|                  | Pore structure characterization of complex lithology reservoir based on NMR |
|                  | logging   |
| 11:40 – 11:55 am | Oral 4: Lu Zhang, China University of Petroleum (Beijing), China,           |
|                  | Temperature sensitivity of NMR porosity                                     |

### **Lunch and Break**

12:00 – 13:30 am

### **Session 12**

### Chair: Jun Xu, Wuhan Institute of Physics and Mathematics

| 13:30 – 14:15 pm | Keynote lecture: Xin Zhou, Wuhan Institute of Physics and            |
|------------------|--|
|                  | Mathematics, Chinese Academy of Sciences, China, Hyperpolarized      |
|                  | Xenon multinuclear and CEST MRI in biomedicine                       |
| 14:15 – 14:40 pm | Invited lecture 1: Hua Guo, Tsinghua University, China, 3D Diffusion |
|                  | MRI using Simultaneous Multi-slab Imaging                            |



14:40 – 15:05 pm Invited lecture 2: Dan Wu, Zhejiang University, China, *Microstructural* 

imaging with diffusion-time-dependent diffusion MRI

15:05 – 16:00 pm Poster Session and Coffee Break

### **Session 13**

### Chair: Chunsheng Zhou, Harbin Institute of Technology, China

| 16:00 – 16:15 pm | Oral 1: Yao Fu, French Alternative Energies and Atomic Energy                |
|------------------|--|
|                  | Commission, France, Revealing hidden defects in Metal-Organic                |
|                  | Frameworks by solid-state NMR  |
| 16:15 – 16:30 pm | Oral 2: Guowen Jin, China University of Petroleum (Beijing), China,          |
|                  | A New Method for Pore Structure Characterization of Porous Rocks Based on    |
|                  | Low Field NMR  |
| 16:30 – 16:45 pm | Oral 3: Xinglong Lei, China University of Petroleum (Beijing), China,        |
|                  | Quantitative evaluation of local porosity and heterogeneity in porous media  |
|                  | with low-field NMR imaging   |
| 16:45 – 17:00 pm | Oral 4: Zhe Zhang, China University of Petroleum (Beijing), China,           |
|                  | Prediction of NMR $T_2$ Spectrum AND $T_2$ CUT-OFF VALUE with Machine        |
|                  | Learning Model   |
| 17:00 – 17:15 pm | Oral 5: Guanghui Shi, China University of Petroleum (Beijing), China,        |
|                  | Automatic optimization of pulse sequence based on closed-loop control        |
|                  | strategy   |
| 17:15 – 17:30 pm | Oral 6: Zhen Xie, China University of Petroleum (Beijing), China,            |
|                  | Numerical simulation study on the influence of temperature on the restricted |
|                  | diffusion in porous media  |
| 17:30 – 17:45 pm | Oral 7: Zijian Jia, University of Shanghai for Science and Technology,       |
|                  | China, Application of artificial intelligence on 2D NMR to identify shale    |
|                  | components   |
| 17:45 – 18:00 pm | Oral 8: Jiangfeng Guo, China University of Petroleum, China,                 |
|                  | Two-dimensional magnetic resonance $T_1$ - $T_2^*$ relaxation correlation    |
|                  | measurements and spectra   |

### Dinner

# FRIDAY, AUGUST 26<sup>TH</sup> 2022 (HYBRID)

金溪山庄,杭州市西湖区杨公堤 39号

### **Session 14**

Chair: Lizhi Xiao, China University of Petroleum, China

| 08:30 – 09:15 am | Keynote lecture: Zhong Chen, Xiamen University, China,                       |
|------------------|--|
|                  | High-resolution NMR spectroscopy for complex chemical and biological         |
|                  | samples  |
| 09:15 – 09:40 am | Invited lecture 1: Chunsheng Zhou, Harbin Institute of Technology,           |
|                  | China, Investigations into moisture-dependent pore structure of cement-based |
|                  | materials through the Low-Field NMR relaxation technique                     |
| 09:40 – 10:05 am | Invited lecture 2: Zheng Xu, Chongqing University, China, A Portable         |
|                  | Shielding-free 50mT Head Magnetic Resonance Imaging System                   |
| 10:05 – 10:30 am | Invited lecture 3: Fangrong Zong, Beijing University of Posts and            |
|                  | Telecommunications, China, Data processing in multi-dimensional NMR          |
|                  | and MRI  |

### **Coffee Break**

10:30 - 10:45 am

### **Session 15**

### Chair: Bingwen Hu, East China Normal University, China

| 8                |  |
|------------------|--|
| 10:45 – 11:00 am | Oral 1: Shuanglan Yan, China University of Petroleum (Beijing),                        |
|                  | China, The Study on NMR Response Mechanism and Evaluation Method of                    |
|                  | Basic Volcanic Rock  |
| 11:00 – 11:15 am | Oral 2: Ruiqi Fan, China University of Petroleum (Beijing), China,                     |
|                  | Quantitative Evaluation Method of Movable Oil Saturation in Shale Oil by               |
|                  | NMR  |
| 11:15 – 11:30 am | Oral 3: Yingyao Qin, Yangtze University, China, <i>Improvement of T<sub>2</sub>-Pc</i> |
|                  | 2D NMR inversion method for characterizing pore-throat connectivity                    |
| 11:30 – 11:45 am | Oral 4: Sihui Luo, China University of Petroleum (Beijing), China, A                   |
|                  | Study on Improving Low-field NMR Echo Data Quality with Dictionary                     |
|                  | Learning   |
| 11:45 – 12:00 am | Oral 5: Gang Luo, China University of Petroleum, China, A Study on                     |
|                  | Multi-exponential Inversion of NMR Relaxation Data with Deep Learning                  |

### **Lunch and Break**

12:00 - 13:30

### **Session 16**

Chair: Luming Peng, Nanjing University, China

| 13:30 – 14:15 pm | Keynote lecture: Wei Wang, Lanzhou University, China, Host-Guest       |
|------------------|--|
|                  | Chemistry of Covalent Organic Frameworks Revealed by Solid-State       |
|                  | NMR Spectroscopy   |
| 14:15 – 14:40 pm | Invited lecture 1: Jun Xu, Wuhan Institute of Physics and              |
|                  | Mathematics, Chinese Academy of Sciences, China, Insight into active   |
|                  | sties and catalytic reactions over metal-zeolites from solid-state NMR |

spectroscopy

14:40 – 15:05 pm **Invited lecture 2**: Guangjin Hou, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China, *Solid-state NMR studies of syngas* 

conversion on oxide-zeolite bifunctional catalysts

manymah

### Coffee Break

15:05 - 15:20 pm

### **Session 17**

### Chair: Yefeng Yao, East China Normal University, China

| 15:20 – 15:45 pm | Invited lecture 3: Luming Peng, Nanjing University, China, Unveiling          |
|------------------|---|
|                  | the surface structure of ZnO nanorods and $H_2$ activation mechanism with 170 |
|                  | NMR spectroscopy  |
| 15:45 – 16:10 pm | Invited lecture 4: Bingwen Hu, East China Normal University, China,           |
|                  | Magnetic resonance for Li-ion battery: from NMR to EPR                        |
| 16:10 – 16:25 pm | Oral 1: Haiming Liu, ShanghaiTech University, China, Structural and           |
|                  | Dynamic Study of MOFs by Solid-State NMR                                      |
| 16:25 – 16:40 pm | Oral 2: Feng Deng, PetroChina Research Institute of Petroleum                 |
|                  | Exploration & Development, China, Magnetic Resonance Flow                     |
|                  | Measurement Method for Petroleum Industry                                     |
| 16:40 – 16:55 pm | Oral 3: Xi Chen, Beijing Limecho Technology Co., Ltd., China,                 |
|                  | Hydration characerization of cement with recycled concrete powder by using    |
|                  | <sup>I</sup> H NMR  |
| 16:55 – 17:10 pm | Oral 4: Jing Qiao, Harbin Institute of Technology, China, Investigation       |
|                  | into the relationship between the compressive strength and pore structure of  |
|                  | saturated white cement mortars  |
| 17:10 – 18:00 pm | Awards & Closing ceremony   |
|                  |   |

### Dinner

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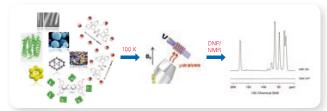


# Solid-State DNP at 263-593 GHz



### Making the Invisible Visible

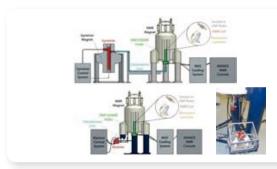
Dynamic Nuclear Polarization (DNP) experiments transfer the high polarization of electron spins to nuclear spins, driven by microwave irradiation of unpaired electron spins. Bruker DNP-NMR spectrometers are designed specifically for extended solidstate NMR experiments, delivering unsurpassed sensitivity and stability for exciting new applications in biological solids, material science and pharmaceuticals.

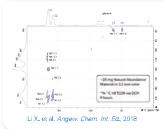


### **Gyrotron and Klystron Microwave Sources**

Bruker's custom-designed gyrotron microwave sources and lowtemperature MAS (LTMAS) probes have a proven record of performance with 53 installed systems to date. We also offer a 263 GHz Extended Interaction Klystron (EIK) with 5 W output power and high frequency/power stability. The 263 GHz klystron provides 80-100% of the gyrotron DNP efficiency (depending on the sample) with a lower purchase price, footprint and facility requirements.

| Magnetic<br>Field | <sup>1</sup> H NMR<br>Frequency | EPR/µwave<br>Frequency | Microwave<br>Source |
|-------------------|---------------------------------|------------------------|---------------------|
| 9.4 T             | 400 MHz                         | 263 GHz                | Klystron            |
| 14.1 T            | 600 MHz                         | 395 GHz                | Gyrotron            |
| 18.8 T            | 800 MHz                         | 527 GHz                | Gyrotron            |
| 21.1 T            | 900 MHz                         | 593 GHz                | Gyrotron            |





Using the 263 GHz klystron, excellent enhancements can be obtained even for highly challenging samples, such as polymeric carbon nitride materials (photocatalysts for solar H, production). With the help of DNP enhancement, 2-dimensional 15N-13C correlation spectra of this material were acquired at natural isotopic abundance in less than 10 hours, allowing the structure of the material to be characterized.

Fig. 1: Polymeric carbon nitride materials doped with 15 mM AMUPol in aqueous solvent yield excellent DNP signal enhancements of 71 with ~5 W of microwave power, allowing 15N-13C correlation spectra to be acquired rapidly even at natural isotopic abundance.

### 1.3 and 1.9 mm MAS DNP Probes

The DNP LTMAS probes operate in the 100-200 K temperature range with cold insert/eject capabilities. They are offered with HCN, HX, HXY (with variety of X/Y combinations) or low gamma RF configuration and the following rotor sizes to cover a range of applications at 400 to 900 MHz:

- 3.2 mm: 15 kHz MAS @ 100 K
- 1.9 mm: 24 kHz MAS @ 100 K
- 1.3 mm: 40 kHz MAS @ 100 K
- 0.7 mm: 65 kHz MAS @ 100 K

The fast MAS probes have optimized microwave coupling into the sample for high DNP efficiency with fast MAS.

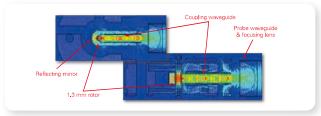


Fig. 2: EM simulations for 1.3 mm optimized DNP stator and waveguide at 263 GHz.

### Fast MAS + DNP

As in conventional solid-state NMR, fast magic angle rotation enables superior decoupling of dipolar interactions, often provides favorable relaxation properties and can even allow for <sup>1</sup>H-detection. Combined with large signal enhancements from DNP, this has opened up new applications in structural biology and materials science.

1.3 mm DNP probes provide ideal sensitivity for limited-quantity samples. As in the case of a  $^{13}\text{C},^{15}\text{N-specifically amino acid labeled dihydrofolate reductase, 4 µL of sample at a concentration of 0.65 mM were sufficient to acquire a <math display="inline">^{1}\text{H-}^{13}\text{C}$ heteronuclear correlation spectrum in just 26 minutes.

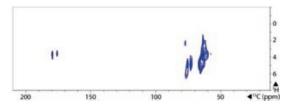


Fig. 3: <sup>1</sup>H-<sup>13</sup>C HETCOR spectrum of specifically-<sup>13</sup>C,<sup>15</sup>N-labeled dihydrofolate reductase at a concentration of only 0.65 mM (2.6 nanomoles of protein in rotor), enhanced with 20 mM TOTAPOL in a 3:7 v/v glycerol-d<sub>g</sub>/D<sub>2</sub>0 buffer, 40 kHz MAS.

### Summary

- Turn-key solution for DNP-enhanced solids NMR experiments at high field.
- Unique high power CW gyrotron microwave sources at 263, 395, 527, 593 GHz.
- Klystron microwave source option at 263 GHz for increased DNP accessibility.
- Low-temperature (100 K) MAS probe technology with built-in waveguide and cold spinning gas supply.
- High DNP signal enhancements on wide range of samples.













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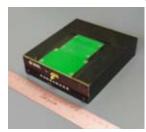
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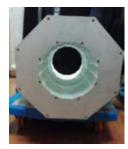
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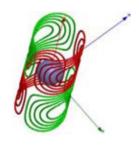
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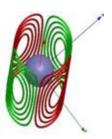
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