



**SSNMR SYMPOSIUM  
JULY 25-29, 2022  
COPPER MOUNTAIN, COLORADO, USA**

**SSNMR SYMPOSIUM COMMITTEE**

David Bryce (Co-Chair)  
Amir Goldbourn (Co-Chair)  
Sophia E. Hayes (Past Chair)  
Tatyana Polenova (Past Chair)  
Marek Pruski (Past Chair)  
Christian Bonhomme  
Björn Corzilius  
Pierre Florian  
Joanna Long  
Rachel Martin  
Ulla Gro Nielsen

**AGENDA**

**MONDAY, JULY 25, 2022**

<b>Pre-Conference Activities</b>	
8:00 AM – 12:30 PM	<b>Bruker SSNMR Symposium</b>
<b>New Methods - David Bryce &amp; Amir Goldbourn presiding</b>	
7:00 PM	Opening Remarks – David Bryce and Amir Goldbourn
7:10 PM	<b>New NMR Approaches for Probing the Structure and Function of Buried Solid Interfaces.</b> Michal Leskes, Weizmann Institute of Science
7:40 PM	<b>Rapid Protein Secondary Structure Determination from a Single Unassigned 1D <sup>13</sup>C NMR Spectrum.</b> Marcus Tuttle, Yale University
8:00 PM	<b>Principles and Developments Towards More Objectivity and Transparency, and More Reliable Sparsity in Nonuniform Sampling.</b> David Rovnyak, Bucknell University
8:30 PM	<b>Millisecond Time-Resolved Solid State NMR: An Approach to Molecular Mechanisms of Folding and Self-Assembly of Biopolymers.</b> Robert Tycko, National Institutes of Health

TUESDAY, JULY 26, 2022

<b>Methods and Materials - Pierre Florian &amp; Ulla Gro Nielsen presiding</b>	
8:20 AM	<b>NMR/MRI Studies of Li Microstructure Formation in Solids.</b> Yan-Yan Hu, Florida State University
8:50 AM	<b>Operando NMR Characterization of Full-Cell Li-ion Batteries Using an Optimized Parallel Plate Resonator.</b> Kevin Sanders, McMaster University
9:10 AM	<b>Less is More: Z-restore Soft-CPMG Approach to Natural Abundance O-17 NMR in Solids.</b> Philip Grandinetti, The Ohio State University
9:30 AM	<b>Understanding the Local Structure of Protective Alumina Coatings for Cathodes and the Coating-Cathode Interface.</b> Abby R. Haworth, Lancaster University
9:50 AM	<i>Break</i>
10:20 AM	<b>Recent Progress in Studying of Materials Surfaces by Conventional and DNP-Enhanced Solid-State NMR.</b> Marek Pruski, Ames Laboratory
10:50 AM	<b>Probing Oxygen Exchange in Metal-organic Frameworks and Their Water Stability Using <sup>17</sup>O NMR.</b> Frédérique Pourpoint, Université de Lille
11:10 AM	<b><sup>27</sup>Al NMR Chemical Shielding and Quadrupolar Tensors Benchmarking with DFT: Machine Learning Prediction of Quadrupolar Coupling Constants (C<sub>q</sub>) from Simple Local Geometry and Elemental Properties.</b> He Sun, Washington University in St. Louis
11:30 AM	<b>Probing Dynamics in Supramolecular Assemblies by Solid-state NMR Spectroscopy.</b> Frédéric Blanc, University of Liverpool
12:00 PM	<i>Lunch (included with registration)</i>
<b>DNP Advances and Applications - Rachel Martin &amp; Marek Pruski presiding</b>	
1:30 PM	<b>Photonic Band-Gap Resonators for DNP of Thin-Film Samples.</b> Alexander Nevzorov, North Carolina State University
2:00 PM	<b>The Role of Methyl Dynamics in DNP.</b> Thomas Biedenbänder, University of Rostock
2:20 PM	<b>MAS Spherical Shell Rotors and Spherical Solenoid Coils Boost RF Homogeneity and NMR Sensitivity.</b> Chukun Gao, ETH Zürich
2:40 PM	<b>Alternative Methods for Generating Endogenous Radicals for High-Field MAS DNP.</b> Scott Carnahan, Ames Laboratory
3:00 PM	<i>Break</i>
3:30 PM	<b>Spotlight DNP: Altering the Distribution of Polarization Agents Highlights Proteins with Different Sub-cellular Localizations.</b> Kendra Frederick, UT Southwestern
4:00 PM	<b>In-Cell Quantification of Drugs by Magic-Angle Spinning Dynamic Nuclear Polarization NMR.</b> Pierrick Berruyer, École Polytechnique Fédérale de Lausanne (EPFL)
4:20 PM	<b>Molecular Architecture and Carbohydrate-Aromatic Interface of Plant Cell Walls Investigated by Solid-state NMR.</b> Wancheng Zhao, Louisiana State University
4:40 PM	<b>Three-Dimensional Structure Determination of a Supported Molecular Catalyst with Multiple Surface Sites.</b> David Gajan, Université de Lyon
5:30-7:00 PM	<i>Conference Reception (included with registration)</i>
<b>Posters</b>	
7:30-9:30 PM	<b>Authors Present for Posters Labeled A</b>

**WEDNESDAY, JULY 27, 2022**

Morning	Free time to explore the area
12:00 PM	<i>Lunch (included with registration)</i>
<b>Vaughan Symposium</b> - David Bryce & Amir Goldbourt presiding	
2:30 PM	Introduction
2:40 PM	<b><i>Vaughan Lecture</i></b> - <b>Biological Solid State NMR: Progress and Potential.</b> Chad Rienstra, University of Wisconsin Madison
3:30 PM	<b>The Activated and Inactivated States of KirBac1.1 Resolved by Solid-state NMR.</b> Benjamin J. Wylie, Texas Tech University
4:00 PM	<i>Break</i>
4:30 PM	<b>Finding the Magic Angle(s) with Undergraduate Research.</b> Kathryn D. Kloepper, Mercer University
5:00 PM	<b>Proton Detection and Very-Fast Magic-Angle Spinning Solid-state NMR as a Tool to Determine the Structures of Complicated Biological Systems.</b> Andrew J. Nieuwkoop, Rutgers University
<b>Posters</b>	
7:30-9:30 PM	<b>Authors Present for Posters Labeled B</b>

THURSDAY, JULY 28, 2022

<b>Integrated Magnetic Resonance I (Joint Session - EPR &amp; SSNMR) - Fraser MacMillan presiding</b>	
<b>IES Fellow Award Presentation</b>	
8:10 AM	<b>Songi Han (IES President) to R. David Britt</b>
8:15 AM	<b>EPR Studies of the Enzymatic Synthesis of the Organometallic H-Cluster of [FeFe] Hydrogenase.</b> R. David Britt, University of California Davis
8:55 AM	<b>Combining Solid-state NMR with DEER EPR to Study Structure and Dynamics of Cross-<math>\beta</math> Fibrils.</b> Ansgar Siemer, University of Southern California
9:15 AM	<b>From Fast Water on Surfaces to Nearly Immobile Nano-Confined Water: Exploring and Expanding the Dynamic Range of Overhauser Dynamic Nuclear Polarization.</b> John M Franck, Syracuse University
9:30 AM	<b>Methyl-Driven Overhauser MAS-DNP.</b> Frédéric Perras, Ames Laboratory
9:50 AM	<i>Break</i>
<b>Integrated Magnetic Resonance II (Joint Session - EPR &amp; SSNMR) - Sophia E. Hayes presiding</b>	
10:15 AM	<b>Up-conversion of Radio-frequency NMR Signals to Light via a Membrane Transducer.</b> Kazuyuki Takeda, Kyoto University
10:45 AM	<b>Spin Textures and Quantum Sensing with Optically Hyperpolarized Nuclei.</b> Ashok Ajoy, University of California Berkeley
11:15 AM	<b>DNP using Spherical Rotors.</b> Lauren Price, ETH Zürich
11:35 AM	<b>Terahertz EPR Spectroscopy Using a 36-Tesla High-Homogeneity Series-Connected Hybrid Magnet.</b> Thierry Dubroca, National High Magnetic Field Laboratory
12:00 PM	<i>Lunch (included with registration)</i>
<b>Biomolecules - Joanna Long &amp; Tatyana Polenova presiding</b>	
1:40 PM	<b>Deuterium Solid-state NMR Methods for Quantification of Protein <math>\mu</math>-ms Time Scales Dynamics.</b> Liliya Vugmeyster, University of Colorado Denver
2:10 PM	<b>Phase States of Prion Protein Coupled to Protein Conformation.</b> Kurt Zilm, Yale University
2:30 PM	<b>NMR-Assisted Crystallography Reveals Hydrogen Atom Positions and Reduced Positional Uncertainties for the Tryptophan Synthase Aminoacrylate Intermediate.</b> Jacob Holmes, University of California Riverside
2:50 PM	<b>Integrated Software Technologies for Biomolecular Solid-state NMR.</b> Woonghee Lee, University of Colorado Denver
3:10 PM	<i>Break</i>
3:40 PM	<b>Combined NMR and HDX-MS Studies Suggest Protein Stabilization is Key to Signaling by Bacterial Chemoreceptor Complexes.</b> Lynmarie Thompson, University of Massachusetts Amherst
4:10 PM	<b>Determination of Accurate <math>^{19}\text{F}</math> Chemical Shift Tensors with R-Symmetry Recoupling at High MAS Frequencies (60-100 kHz).</b> Gal Porat-Dahlerbruch, University of Delaware
4:30 PM	<b>Probing Watson-Crick and Hoogsteen Base Pairing in Duplex DNA using DNP Solid-state NMR.</b> Daniel Conroy, The Ohio State University
4:50 PM	<b>Signaling in Biological Systems -- Insights from NMR.</b> Ann McDermott, Columbia University
7:00-9:00 PM	<i>Conference Banquet &amp; Awards Ceremony (Enjoy an evening of comradeship, fine food and recognition of peers. Pre-registration required.)</i>
8:00 PM	<b>Welcoming Remarks.</b> Kurt Zilm, Conference Chair
8:05 PM	<b>In the Beginning.... It's all about Electronic Structure and Molecular Dynamics.</b> Cynthia Jameson, University of Illinois at Chicago
8:35 PM	EPR Awards
8:45 PM	SSNMR Awards

FRIDAY, JULY 29, 2022

Materials and Methods - David Bryce & Amir Goldbourn presiding	
8:50 AM	<b>Indirect Satellite-transition Detection of <math>^{33}\text{S}</math> and <math>^{17}\text{O}</math> at Natural Abundance by Progressive Saturation of the Proton Reservoir (PROSPR).</b> Tamar Wolf, Weizmann Institute of Science
9:10 AM	<b>Modeling and Optimization of Multiple-Quantum Magic-Angle Spinning NMR Spectra.</b> Lexi McCarthy, The Ohio State University
9:30 AM	<b>Modelling NMR Properties of Oxide Glasses with Machine Learning.</b> Thibault Charpentier, Université Paris-Saclay
10:00 AM	<i>Break</i>
10:30 AM	<b>Scalable Nanoporous Networks for <math>\text{CO}_2</math> Chemisorption via Solid-state NMR Spectroscopy.</b> Haiyan Mao, University of California Berkeley
10:50 AM	<b>Investigating Structure and Dynamics in Solar Thermal Fuels by Solid-state NMR.</b> John Griffin, Lancaster University
11:10 AM	<b>NMR Crystallography and Crystal Structure Prediction using Quadrupolar Nuclei (QNMRX-CSP).</b> Carl Fleischer, III, Florida State University
11:30 AM	<b>Exploiting <math>^{17}\text{O}</math> Isotopic Enrichment in NMR Spectroscopy of Microporous Materials.</b> Sharon Ashbrook, University of St Andrews
12:00 PM	Closing remarks