



**SSNMR SYMPOSIUM**  
**JULY 17-21, 2016**  
**BRECKENRIDGE, COLORADO, USA**

**SSNMR SYMPOSIUM COMMITTEE**

Gillian Goward (Co-Chair)  
Leonard Mueller (Co-Chair)  
Gerard Harbison (Past Chair)  
Ulrich Scheler (Past Chair)  
Sharon Ashbrook  
David Bryce  
Sophia E. Hayes  
Christopher Jaroniec  
Joanna Long  
Tatyana Polenova  
Marek Pruski

**AGENDA**

**SUNDAY, JULY 17, 2016**

<b>Pre-Conference Activities</b>	
9:00 AM-1:00 PM	<b>Bruker Solid-State NMR Workshop and Seminar</b>
<b>Materials/NMR Crystallography - Gillian Goward presiding</b>	
7:00 PM	Opening Remarks - Gillian Goward and Leonard Mueller
7:10 PM	<b>Solid-State NMR Analyses of Order and Disorder in Rare-earth-doped Oxide Phosphors.</b> Bradley Chmelka, University of California Santa Barbara
7:40 PM	<b>Higher Accuracy Solid-State NMR Chemical Shift Predictions at Lower Computational Cost.</b> Gregory Beran, University of California Riverside
8:00 PM	<b>Distinguishing Faceted Oxide Nanocrystals with <sup>17</sup>O Solid-State NMR Spectroscopy.</b> Luming Peng, Nanjing University
8:20 PM	<b>NMR Crystallography for Analyzing Selective Host-Guest Interactions in Metal-Organic Frameworks.</b> Juergen Senker, University of Bayreuth

MONDAY, JULY 18, 2016

<b>Biomethods and Biomolecules - Leonard Mueller &amp; Chris Jaroniec presiding</b>	
8:20 AM	Opening Remarks
8:30 AM	<b>Gaining More Systems to Solid-State NMR.</b> Claudio Luchinat, CERM - University of Florence
9:00 AM	<b>Analysis of Local Dynamics in Proteins Using CP-VC Under Ultra-fast MAS.</b> Jean Paul Amoureux, Lille University
9:30 AM	<b>Insight into Dynamic Regulation of HIV-1 Maturation with an Integrated Magic Angle Spinning NMR and Molecular Dynamics Approach.</b> Caitlin Quinn, University
10:00 AM	<i>Break</i>
10:30 AM	<b>Solid-State NMR Studies of Peroxidase-active Membrane-bound Cytochrome c - A Pivotal Trigger of Mitochondrial Apoptosis.</b> Patrick van der Wel, University of Pittsburgh
11:00 AM	<b>Structural Virology of Filamentous Bacteriophages – The Effect of a Single Coat Protein Mutation Through Three Length Scales.</b> Amir Goldbourn, Tel Aviv University
11:20 AM	<b>High-Resolution Solid-State NMR Structure of a Pathogenic Fibril of <math>\alpha</math>-Synuclein Fibrils.</b> Marcus D. Tuttle, Yale University
11:40 AM	<b>Structural Investigations of a Functional Amyloid Important for Long-term Memory.</b> Ansgar Siemer, University of Southern California
12:00 PM	<i>Lunch (included with registration)</i>
<b>Materials &amp; Methods - Sharon Ashbrook &amp; Marek Pruski presiding</b>	
1:30 PM	<b>Topological Band Structures Probed by NMR.</b> Louis Bouchard, UCLA
2:00 PM	<b>Solid-State NMR Proves the Presence of 5-fold Coordinated Scandium in Metal-Organic Frameworks.</b> Frédérique Pourpoint, UCCS - ENSCL - University of Lille
2:20 PM	<b>Exploring Wedsleyite Hydration by Combining AIRSS and NMR Spectroscopy.</b> Robert F. Moran, University of St. Andrews
2:35 PM	<b>DNP Enhanced Solid-State NMR Spectroscopy of Heterogeneous Catalysts.</b> David Gajan, ISA-CRMN
2:50 PM	<b>Structural and Dynamics Investigation of new fast Li ion conductors using Solid-State NMR Spectroscopy.</b> Kenneth K. Inglis, University of Liverpool
3:05 PM	<i>Break</i>
<b>Materials &amp; Methods (continued) - Sharon Ashbrook &amp; Marek Pruski presiding</b>	
3:30 PM	<b>Interfaces in Polymer Hybrid Materials.</b> Ulrich Scheler, Leibniz-Institut für Polymersforschung Dresden e.V.
4:00 PM	<b><sup>7</sup>Li MATPASS NMR Spectroscopy Combined with Monte Carlo Simulations for Structure Solution of Metal-Oxide Li Battery Cathodes.</b> Kris Harris, McMaster University
4:15 PM	<b>Charging Mechanisms and Dynamics in Supercapacitors.</b> Alexander C. Forse, University of Cambridge
4:30 PM	<b>Solid-State NMR Studies of Rechargeable Battery Materials.</b> Yan-Yan Hu, Florida State University. National High Magnetic Field Laboratory
4:50 PM	<b>Studying the Effects of Metallic Nanoparticles on Conversion Negative Electrode Materials using Solid-State NMR.</b> Karen E. Johnston, Durham University
5:30-7:00 PM	<i>Conference Reception</i>
<b>Posters</b>	
7:30-9:30 PM	<b>Authors Present for Posters Labeled A</b>

TUESDAY, JULY 19, 2016

Morning	Free time to explore the area
12:00 PM	<i>Lunch (included with registration)</i>
<b>Vaughan Symposium - Materials &amp; Quadrupolar NMR - Gillian Goward &amp; Leonard Mueller presiding</b>	
1:20 PM	Introduction
1:30 PM	<b>Vaughan Lecture - Local and Medium Range Order and Disorder as Viewed by NMR: Concepts, Methods and Applications.</b> Dominique Massiot, CNRS
2:15 PM	<b>On The Potential of Optically-pumped and Microwave-driver DNP of Diamonds in Solid-State and Dissolution<sup>13</sup> CNMR.</b> Lucio Frydman, Weizmann Institute
2:45 PM	<b>Methodological Developments in Solid-State NMR with Applications in Catalysis and Energy Materials.</b> Arno Kentgens, Radboud University
3:15 PM	<i>Break</i>
4:00 PM	<b>Combined Solid-State NMR and Molecular Dynamics Investigation of the Structure of Sr-, Ba- or Zn-Aluminosilicate Glasses.</b> Pierre Florian, CEMHTI-CNRS
4:20 PM	<b>2D NMR Measurement and Prediction of Full Paramagnetic Shift Tensors of Quadrupolar Nuclei.</b> Philip J. Grandinetti, Ohio State University
4:50 PM	<b>Looking into the Structure and Reactivity of Hybrid Materials Involving Boronates and Benzoxaborolates.</b> Danielle Laurencin, Université de Montpellier
5:20-7:20 PM	<i>CortecNet Reception</i>
<b>Posters</b>	
7:30-9:30 PM	<b>Authors Present for Posters Labeled B</b>

WEDNESDAY, JULY 20, 2016

<b>Integrated Magnetic Resonance I. (Joint Session - EPR &amp; SSNMR) - Sophia Hayes &amp; John Morton presiding</b>	
8:15 AM	<b>Towards Spin-assisted Long-term Data Storage in Diamond.</b> Carlos Meriles, CUNY - City College of New York
8:45 AM	<b>Electron Spectral Diffusion Measured via ELDOR for DNP at 7 T.</b> Alisa Leavesley, University of California Santa Barbara
9:00 AM	<b>Hypersensitivity with Dynamic Nuclear Polarization: Natural Isotopic Abundance and Closed-loop Cryogenic Helium Sample Spinning.</b> Gaël De Paëpe, INAC (CEA - Grenoble Alpes University)
9:30 AM	<b>Combining Dynamic Nuclear Polarization and Mechanically Detected Magnetic Resonance to Achieve Nanoscale Magnetic Resonance Imaging of Individual Biomolecules and Assemblies.</b> John Marohn, Cornell University
9:45 AM	<b>Electron Spin Decoupled NMR Driven by Electron Spin Relaxation of Spin Clusters.</b> Ting Ann Siaw, University of California Santa Barbara
10:00 AM	<i>Break</i>
<b>Integrated Magnetic Resonance II. (Joint Session - EPR &amp; SSNMR) - Sophia Hayes &amp; John Morton presiding</b>	
10:40 AM	<b>Nanoscale NMR Detection and Imaging Using Nitrogen-vacancy Centers in Diamond.</b> Daniel Rugar, IBM Almaden Research Center
11:10 AM	<b>Technology for Hyperfine Decoupling and Time Domain DNP in Rotating Solids.</b> Alexander Barnes, Washington University in St. Louis
11:25 AM	<b>Nuclear Magnetic Resonance Spectroscopy on a Nanostructured Diamond Chip for Chemical Trace Analysis.</b> Nazanin Mosavin, CHTM-UNM
11:40 AM	<b>Gd<sup>3+</sup> as Polarizing Agent at High Field: Solid Effect vs Cross Effect Dynamic Nuclear Polarization.</b> Monu Kaushik, Goethe University Frankfurt
12:00 PM	<i>Lunch (included with registration)</i>
<b>Bio-Methods/DNP - Joanna Long &amp; Tatyana Polenova presiding</b>	
1:15 PM	<b>Advancing NMR of Membrane Proteins in the Lipid Bilayer Membrane.</b> Francesca Marassi, Sanford Burnham Prebys Medical Discovery Institute
1:45 PM	<b>Effect of the Lipid Composition and Bilayer Viscosity on the Structure and Dynamics of Nanopore-Aligned Membrane Proteins as Revealed by Solid-State NMR.</b> Alexander Nevzorov, North Carolina State University
2:05 PM	<b>Magic Angle Spinning Solid State NMR Studies of Membrane Proteins in Synthetic Lipids and Cell Membranes.</b> Vladimir Ladizhansky, University of Guelph
2:35 PM	<b>Solid-State 15N- and 19F-NMR Analysis of the Interaction of the Viral E5 Oncoprotein with the PDGF Receptor in Membranes.</b> Dirk Windisch, Karlsruhe Institute of Technology
3:05 PM	<i>Break</i>
<b>Bio-Methods/DNP (continued) - Joanna Long &amp; Tatyana Polenova presiding</b>	
3:40 PM	<b>EPR and DNP in the Same Probe: Optimizing Microwave Delivery to Small Samples for Low Power DNP.</b> Kurt W. Zilm, Yale University
4:00 PM	<b>Solid-State NMR, DNP, and MD Investigations of the Organic/Inorganic Interface in Silica Biohybrids.</b> Stephan Brückner, TU Dresden
4:20 PM	<b>A Hidden Mode of Action of Glycopeptide and Cyclopeptide Antibiotics Determined by <sup>13</sup>C{<sup>15</sup>N} and <sup>15</sup>N{<sup>13</sup>C}REDOR NMR.</b> Sung Joon Kim, Baylor University
4:40 PM	<b>The Polymeric Skin of Potatoes: Molecular Insights into Plant Defense from Solid-State NMR.</b> Ruth E. Stark, CUNY City College of New York
5:10 PM	<b>Energy Landscapes, Anisotropic Motions and Dynamics in Large Protein Complexes.</b> Józef R. Lewandowski, University of Warwick
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>
7:55 PM	<b>Welcoming Remarks.</b> Kurt Zilm, Conference Chair
8:00 PM	<b>Half Century of Unconventional Paths in Magnetic Resonance: Rear View Mirror of a Former Solid-State NMR'er.</b> Eiichi Fukushima, New Mexico Resonance
8:30 PM	EPR Awards
8:40 PM	SSNMR Awards

THURSDAY, JULY 21, 2016

<b>Bio-Molecules/Materials - Chris Jaronic &amp; Marek Pruski presiding</b>	
9:00 AM	<b>Deuterium NMR Spectroscopy for Structure and Dynamics of Protein.</b> Umit Akbey, Aarhus University
9:20 AM	<b>Quadruple-resonance <math>^1\text{H}/^{13}\text{C}/^2\text{H}/^{15}\text{N}</math> MAS Probe for Structure Determination of Extensively Deuterated Biomolecular Solids.</b> Rachel Martin, University of California Irvine
9:40 AM	<i>Break</i>
10:10 AM	<b>Using <math>^1\text{H}</math> <math>T_1</math> Relaxation Times for Measuring Particle Size, Purity, and Stability of Crystalline Organic Compounds.</b> Eric J. Munson, University of Kentucky
10:30 AM	<b>The Importance of Allowing Quadrupolar Polarization of the Core in the Computation of Electric Field Gradients.</b> Gerard R. Harbison, University of Nebraska at Lincoln
11:00 AM	<b>New Frontiers in <math>^{14}\text{N}</math> Solid-State NMR.</b> Robert W. Schurko, University of Windsor
11:20 AM	<b>100+ kHz MAS Solid-State NMR for Natural Abundance Samples.</b> Yusuke Nishiyama, JEOL Resonance, Inc.
11:50 AM	Closing remarks and 2018 Vaughan Lecturer Call for Nominations