



**SSNMR SYMPOSIUM
JULY 13-17, 2014
COPPER MOUNTAIN, COLORADO, USA**

SSNMR SYMPOSIUM COMMITTEE

Gerard Harbison (Chair)
Ulrich Scheler (Chair)
Zhehong Gan (Past Chair)
Rob Schurko (Past Chair)
Sharon Ashbrook
Gillian Goward
Sophia E. Hayes
Christopher Jaroniec
Leonard Mueller
Tatyana Polenova
Marek Pruski

AGENDA

SUNDAY, JULY 13, 2014

Pre-Conference Activities	
9:00 AM-12:20 PM	Bruker Solid-State NMR Workshop and Seminar
1:00 PM-3:30 PM	Viewing of World Cup Final <i>Incline Bar & Grill</i> (food discount and limited reserved seating if wearing your RMCMR badge)
G.S. Harbison presiding	
7:00 PM	Opening Remarks - Gerard Harbison
7:10 PM	Calculations of Indirect Spin-spin (J) Couplings in the Solid-state. Jonathan Yates, University of Oxford
7:40 PM	ZORA/DFT Investigations of NMR Parameters for Solid Materials Containing Heavy Nuclei. Fahri Alkan, University of Delaware
8:00 PM	Extending CPMG Beyond Static Two-Level Systems. Zhehong Gan, NHMFL
8:30 PM	Relaxation-Assisted Separation of Overlapping Patterns in Ultra-Wideline NMR Spectroscopy. Michael Jaroszewicz, University of Windsor
8:50 PM	<i>Gary Maciel Eulogy</i>

MONDAY, JULY 14, 2014

T. Polenova presiding	
8:30 AM	Structural Investigations of Curvature-Inducing Viral Membrane Proteins and Cryoprotected Lipid Membranes at Low Temperature by Solid-State NMR. Mei Hong, Iowa State University
9:00 AM	Structural Restraints and Mechanistic Insights from ¹³C, ¹⁵N, and ³¹P NMR Spectroscopy of the Enzyme Active Site in Tryptophan Synthase. Bethany Caulkins, University of California Riverside
9:20 AM	Inactivation and Allostery in a Potassium Channel. Ann McDermott, Columbia University
9:50 AM	<i>Break</i>
10:20 AM	Heavy Mice and Lighter Things: Using Solid-State NMR to Map Molecular Structures in Tissues. Melinda Duer, University of Cambridge
10:50 AM	NMR and EPR Studies of Protein-mediated Lipid Organization, Structure, and Dynamics in Lung Surfactant. Joanna Long, University of Florida
11:10 AM	Amphotericin Forms a Sterol Sponge That Kills Yeast Primarily by Extracting Ergosterol From the Lipid Bilayer. Chad Rienstra, University of Illinois
11:30 AM	Solid-State NMR of Multispan Membrane Proteins and Membrane Protein Complexes. Gianluigi Veglia, University of Minnesota
12:00 PM	<i>Lunch (included with registration)</i>
L. Mueller presiding	
1:30 PM	New Development in High-Field Protein Solid-State NMR using Ultra-Fast MAS and Structural Insights into Brain-derived Amyloid-β Oligomers. Yoshitaka Ishii, University of Illinois Chicago
1:50 PM	The Intrinsic Conformational Plasticity of Native EmrE Using Solid-State NMR Spectroscopy. Nate Traaseth, New York University
2:10 PM	High Resolution ¹H-detected Solid-State NMR With Fast Magic-angle Spinning: From Microcrystalline Proteins to Large Protein Assemblies. Guido Pintacuda, Université de Lyon
2:40 PM	A Solid State ³¹P and ²⁹Si MAS NMR, ⁴³Ca DOR NMR, and GIPAW DFT Study of α-Tricalcium Phosphate and Si-Substituted α-Tricalcium Phosphate Bioactive Materials. John V. Hanna, University of Warwick
3:00 PM	<i>Break</i>
C. Jaroniec presiding	
3:30 PM	Synthetic Substituted Hydroxyapatites: New Insight by DNP MAS Spectroscopy and New Avenues for Natural Samples. Christian Bonhomme, Université Pierre et Marie Curie
4:00 PM	Role of Electron Spin Dynamics on Solid-State Dynamic Nuclear Polarization Performance. Songi Han, University of California Santa Barbara
4:20 PM	Determining the Conformation of Surface Species by DNP Enhanced Solid-State NMR. Anne Lesage, University of Lyon
4:50 PM	Dynamic Nuclear Polarization Enhanced Solid State NMR of Oxygen-¹⁷ at Natural Abundance and Other Insensitive Nuclei. Frederic Blanc, University of Liverpool
5:30-7:00 PM	<i>Conference Reception</i>
Posters	
7:30-9:00 PM	Authors Present for Posters Labeled A

TUESDAY, JULY 15, 2014

Morning	Free time to explore the area
12:00 PM	<i>Lunch (included with registration)</i>
Vaughan Symposium - U. Scheler presiding	
1:30 PM	Award Presentation
1:45 PM	<i>Vaughan Lecture - Furthering Our Understanding of the Fundamental NMR Parameters and Applying This Knowledge to Investigate Molecular Structure and Dynamics.</i> Roderick E. Wasylshen, University of Alberta
2:25 PM	The Chemical Shift Tensor of Xenon in Nanochannels of Crystalline Solids. Cynthia J. Jameson, University of Illinois Chicago
3:05 PM	<i>Break</i>
3:35 PM	Predictions of NMR Chemical Shifts in Heavy-element Compounds: Giant Spin-orbit Shifts and More. Martin Kaupp, Technical University of Berlin
4:15 PM	New Advances in Ultra-Wideline Solid-State NMR. Robert W. Schurko, University of Windsor
5:30-7:00 PM	<i>SSNMR Hors D'oeuvre reception</i>

WEDNESDAY, JULY 16, 2014

Joint EPR-SSNMR Symposium, S. Han & U. Scheler presiding	
8:15 AM	Dynamic Nuclear Polarization: Electrons and Nuclei and What's in Between. Shimon Vega, Weizmann Institute of Science
8:45 AM	Overhauser Dynamic Nuclear Polarization in Insulating Solids. Robert Griffin, MIT
9:15 AM	What Can DNP Learn From High Field EPR? Graham Smith, University of St. Andrews
9:40 AM	Challenges in Adapting Pulsed Field Gradients and DNP to Fast MAS Solid-State NMR. Kurt Zilm, Yale University
10:05 AM	<i>Break</i>
M. Pruski presiding	
10:35 AM	Towards Natural Abundance C-N Correlations: DNP-Enhanced 14N Overtone Spectroscopy. Luke O'Dell, Deakin University
10:55 AM	15N Solid-State NMR Studies of Hydrogen Storage Media Using Dynamic Nuclear Polarization, Fast Magic Angle Spinning and Computational Methods. Takeshi Kobayashi, Ames National Lab
11:15 AM	Two Complementary Methods to Improve NMR Sensitivity: Dynamic Nuclear Polarization and Non-Uniform Sampling. Olivier Lafon, University of Lille
12:00 PM	<i>Lunch (included with registration)</i>
G. Goward presiding	
1:30 PM	MAS-NMR, Diffusion and Relaxation Properties of Materials for Lithium Batteries. Michael Deschamps, Université d'Orléans
2:00 PM	Developments and Investigations on Battery Materials. Raiker Witter, University of Tallinn
2:20 PM	New NMR, PFG and MRI Methods for Studying Structure and Dynamics in Batteries and Supercapacitors. Clare Grey, University of Cambridge
2:50 PM	<i>Break</i>
S. Hayes presiding	
3:20 PM	Recoupling of Homonuclear Dipole-Dipole Interactions in High-Resolution NMR Spectra of Multispin Systems: Applications to Inorganic Materials. Hellmut Eckert, Westfälische Wilhelms-Universität Münster
3:50 PM	Biomimetic Interplay of Phosphate and Water in Tuning Amorphous CaCO₃ Metastability: Stabilization vs. Spontaneous Phase Separation and Crystallization. Asher Schmidt, Technion-Israel Institute of Technology
4:10 PM	Exploring Local Structure and Surface Chemistry of Ceria Nanoparticles With 17O Solid-State NMR Spectroscopy. Luming Peng, University of Nanjing
4:30 PM	Vol'kenshtein Bundles: Understanding the Connection Between Mechanical Properties and Molecular Structure in Polycarbonate-like Glasses. Jacob Schaefer, Washington University
5:00 PM	Heteronuclear NMR as surface-selective technique: A Unique Look on the Hydroxyl Groups of γ-alumina. Laurent Delevoye, ENSC-Lille
Posters	
7:30-9:00 PM	Authors Present for Posters Labeled B

THURSDAY, JULY 17, 2014

S. Ashbrook presiding	
8:30 AM	Structural Information on Quadrupolar/spin-1/2 pairs Obtained by Phase Modulated Pulses. Amir Goldbourt, Tel Aviv University
8:50 AM	Homonuclear J Coupling Between Quadrupolar Nuclei Measured Using an Ultra-Wideline 2D J-Resolved Experiment. A Direct Probe of Metal-Metal Bonding. Frederic Perras, University of Ottawa
9:10 AM	Synchrotron Powder Diffraction and Solid-State NMR Spectroscopy: Structure Resolution of Metal-Organic-Frameworks Based on Naturally Occurring Linkers. Charlotte Martineau, University of Versailles
9:30 AM	TBA. Jörn Schmedt auf der Günne, Siegen University
10:00 AM	<i>Break</i>
10:30 AM	Deuterium SSNMR as a Probe of Solvate and Hydrate Formation in Pharmaceutical Solids. Jason Ash, Merck Center for Science and Engineering
10:50 AM	Molecular Motions in Different Solid Phases of Organic Ionic Plastic Crystal. Haijin Zhu, Deakin University
11:10 AM	Paramagnetic ^{15}N Shifts from Iron Ion in Nitrogen-Doped Carbon ORR Active Electrochemical Catalysts for PEFC. Shigeki Kuroki, University of Tokyo
11:30 AM	Closing remarks