ROCKY MOUNTAIN CONFERENCE
ON MAGNETIC RESONANCE

SSNMR SYMPOSIUM
JULY 22-26, 2018
SNOWBIRD, UTAH, USA

SSNMR SYMPOSIUM COMMITTEE

Sharon Ashbrook (Co Chair)
Christopher Jaroniec (Co Chair)
Gillian Goward (Past Chair)
Leonard Mueller (Past Chair)
Christian Bonhomme
David Bryce
Amir Goldbourt
Sophia E. Hayes
Joanna Long
Tatyana Polenova
Marek Pruski

AGENDA

SUNDAY, JULY 22, 2018

Pre-Conference Activities	
9:00 AM – 3:00 PM	**Bruker Solid-state NMR Workshop and Seminar**
Materials and Biomaterials - Christopher Jaroniec & Sharon Ashbrook presiding	
7:00 PM	Opening Remarks – Christopher Jaroniec and Sharon Ashbrook
7:10 PM	**Protein Dynamics: Thermal and Driven Motion.** Beat Meier, ETH Zurich
7:40 PM	**Solid-State NMR as a Probe of Donor-Acceptor Interactions in Organic Materials.** John Griffin, Lancaster University
8:00 PM	**Acellular vs Cellular Bone Minerals - Differences Inferred from Modified MAS NMR Techniques.** Gil Goobes, Bar Ilan University
8:20 PM	***In-Situ* Mapping of Li Concentration in Graphite Electrodes by Magnetic Resonance Techniques.** Gillian Goward, McMaster University

MONDAY, JULY 23, 2018

Materials – Sophia Hayes & Marek Pruski presiding	
8:30 AM	**Relayed DNP for Inorganic Solids.** Lyndon Emsley, EPFL
9:00 AM	**Tracing Dynamic Nuclear Polarization Pathways with Transition Metal-Nuclear Spin Rulers.** Sheetal Jain, University of California, Santa Barbara
9:20 AM	**Local Geometries and Electronic Structure in Paramagnetic Materials Revealed by 60-111 kHz MAS NMR Spectroscopy and DFT Calculations.** Kevin Sanders, Université de Lyon
9:40 AM	**36 T Series-Connected-Hybrid Magnet for NMR Spectroscopy at NHMFL.** Xiaoling Wang, National High Magnetic Field Laboratory
10:00 AM	*Break*
10:30 AM	**Mechano- and Vapo-chromic Luminescent Materials: Insights from High-resolution Solid-state NMR Spectroscopy.** Charlotte Martineau-Corcos, ILV & CEMHTI
11:00 AM	**Recent Advances in Atomic-Scale Characterization of Single-Site Heterogeneous Catalysts by Fast-MAS and DNP-Enhanced SSNMR.** Takeshi Kobayashi, US DOE Ames Laboratory
11:20 AM	**Investigating the Mechanism and Electronic Properties of Electrochemically Metallised VO_2 using Solid-State NMR.** Michael Hope, University of Cambridge
11:40 AM	**Resolving Structural Ambiguities in Layered Double Hydroxides by Solid-State NMR.** Ulla Gro Nielsen, University of Southern Denmark
12:00 PM	*Lunch (included with registration)*
Biomolecules – Tatyana Polenova & Joanna Long presiding	
1:30 PM	**NMR Instrumentation for Semi-solid Biological Samples: Development and Application to Hydrogels and Liquid Droplets of Eye Lens Proteins.** Rachel Martin, University of California Irvine
2:00 PM	**Structure of α-Synuclein Fibrils Derived from Parkinson's Disease Dementia Brain Tissue.** Alexander Barclay, University of Illinois at Urbana-Champaign
2:20 PM	**Structural Fingerprinting of Neurotoxic Protein Aggregates at Natural Isotopic Abundance by DNP-Enhanced Solid-State NMR: Towards Patient Derived Structural Measurements.** Adam Smith, CEA Grenoble
2:40 PM	**Closing the Structural Design Loop for Self-Assembling Peptides and Peptide Mimics with Solid-State NMR.** Anant Paravastu, Georgia Institute of Technology
3:00 PM	*Break*
3:30 PM	**^{19}F NMR of Crystalline Tryptophans and HIV-1 Capsid Assemblies.** Angela Gronenborn, University of Pittsburgh
4:00 PM	**Peptide-Based Biradicals for Dynamic Nuclear Polarization of Solid-State NMR Spectroscopy.** Daniel Conroy, The Ohio State University
4:20 PM	**Analysis of a Bacteriophage Tail-Tube Assembly by Proton-Detected Solid-State NMR: Combination of 4D Assignment Experiments and Methyl Labeling.** Maximilian Zinke, FMP Berlin
4:40 PM	**Fast Magic-Angle-Spinning ^{19}F Spin Exchange NMR for Determining Nanometer Distances in Proteins and Pharmaceutical Compounds.** Matthias Roos, Massachusetts Institute of Technology
5:30-7:00 PM	*Conference Reception (included with registration)*
Posters	
7:30-9:30 PM	**Authors Present for Posters Labeled A**

TUESDAY, JULY 24, 2018

Morning	Free time to explore the area
12:00 PM	*Lunch (included with registration)*
Vaughan Symposium – Sharon Ashbrook & Christopher Jaroniec presiding	
2.30 PM	Introduction
2:40 PM	***Vaughan Lecture*** **- Nondestructive Testing of Materials by Compact NMR.** Bernhard Blumich, RWTH Aachen University
3:30 PM	**How to Avoid the Competition with B. Blümich: NMR Spectroscopy of Inorganic Materials Using Large High-field Magnets.** Olivier Lafon, University of Lille
4:00 PM	*Break*
4:30 PM	**Liquid and Gas Diffusion in Metal-Organic Frameworks.** Jeffrey Reimer, University of California, Berkeley
5:00 PM	**Dynamic Polarization of ^{13}C Spins via Nitrogen-Vacancy Centers in Diamond.** Carlos Meriles, CUNY - City College of New York
Posters	
7:30-9:30 PM	**Authors Present for Posters Labeled B**

WEDNESDAY, JULY 25, 2018

Integrated Magnetic Resonance I. (*Joint Session - EPR & SSNMR*) Sophia Hayes & Gail Fanucci presiding	
8:05 AM	**Time Domain Dynamic Nuclear Polarization (and Some CW Experiments on Proteins).** Robert G. Griffin, Massachusetts Institute of Technology
8:35 AM	**Characterizing Microwave Efficiency in DNP Instrumentation by Frequency Swept EPR.** Anne M. Carroll, Yale University
8:55 AM	**Cavity-free 9.4 Tesla EPR Spectrometer for Large Samples used in DNP Experiments.** Jean-Philippe Ansermet, Ecole Polytechnique Fédérale de Lausanne
9:25 AM	**Magic Angle Spinning Spheres, Electron Decoupling with CPMAS Below 6 K, and DNP within Human Cells Using Fluorescent Polarizing Agents.** Alexander B. Barnes, Washington University in St. Louis
9:45 AM	*Break*
Integrated Magnetic Resonance II. (*Joint Session - EPR & SSNMR*) Sophia Hayes & Gail Fanucci presiding	
10:15 AM	**Novel Aspects of Polarization Propagation and Biomolecular Applications of MAS DNP.** Björn Corzilius, Goethe University
10:45 AM	**Truncated Cross Effect Dynamic Nuclear Polarization: Overhauser Effect Doppelgänger.** Asif Equbal, University of California Santa Barbara
11:05 AM	**Breaking Concentration Sensitivity Barrier by Larger Volumes: Photonic Band-Gap Resonators for mm-Wave EPR and DNP of Microliter-Volume Samples.** Alex I. Smirnov, North Carolina State University
11:35 AM	**Optical Room Temperature ^{13}C Hyperpolarization in Powdered Diamond.** Ashok Ajoy, University of California Berkeley
12:00 PM	*Lunch (included with registration)*
Materials and Methodology – Christian Bonhomme & David Bryce presiding	
2:00 PM	**NMR Crystallography of Disorder in Molecular Organics.** Paul Hodgkinson, Durham University
2:30 PM	**In Situ DNP NMR Investigation of Metastable Polymorphs of Glycine.** Giulia Mollica, Aix Marseille Université
2:50 PM	**DNP-NMR Spectroscopy Using a 263 GHz Integrated THz System.** Thorsten Maly, Bridge12 Technologies Inc
3:10 PM	**Trajectory-Based Simulation Approach for the Analysis of Solid-State Exchange Experiments Aimed to Complex Motional Models.** Detlef Reichert, University of Halle
3:30 PM	*Break*
4.00 PM	**Metal-Organic Frameworks: a Playground for Solid-State NMR.** Yining Huang, The University of Western Ontario
4:30 PM	**Refining Crystal Structures with Quadrupolar NMR and Dispersion-Corrected Density Functional Theory.** Sean Holmes, University of Windsor
4:50 PM	**A Combined NMR, First Principles and Monte Carlo Study of the Impact of Fluorine Doping on the Local Structure and Electrochemistry of the $Li_{1.15}Ni_{0.45}Ti_{0.3}Mo_{0.1}O_{1.85}F_{0.15}$ Lithium-Ion Cathode.** Raphaele Clement, University of California, Berkeley
5:10 PM	**Local Structure and Reactivity of Hydrogen-Bonded and Non-Hydrogen-Bonded Brønsted Acid Sites in Zeolites.** Hubert Koller, University of Muenster
7:00-9:00 PM	Conference Banquet & Awards Ceremony *(Enjoy an evening of comradeship, fine food and recognition of peers. Pre-registration required.)*
7:55 PM	**Welcoming Remarks.** Kurt Zilm, Conference Chair
8:00 PM	***A Half Century of RF, µw's and the Magic Angle*.** Robert G. Griffin, Massachusetts Institute of Technology
8:30 PM	EPR Awards
8:40 PM	SSNMR Awards

THURSDAY, JULY 26, 2018

Materials and Biomolecules – Amir Goldbourt presiding	
8.30 AM	**Characterization of Inorganic and Organic Materials by Sensitivity-Enhanced Solid-State NMR Spectroscopy.** Aaron Rossini, Iowa State University
9:00 AM	**Heteronuclear Cross-Relaxation Under Solid-State Dynamic Nuclear Polarization of Biomolecular Complexes.** Victoria Aladin, Goethe University
9:20 AM	**Revealing the Supramolecular Architecture of Fungal Cell Walls Using DNP Solid-State NMR.** Tuo Wang, Louisiana State University
9:40 AM	**^{19}F Solid-State Dynamic Nuclear Polarization Enhanced NMR.** Jasmine Viger-Gravel, EPFL
10:00 AM	*Break*
Biomolecules – Amir Goldbourt & Christopher Jaroniec presiding	
10:30 AM	**The Structural Basis of Cross-seeding Between Phosphorylated and Wild-type β-amyloid Fibrils.** Wei Qiang, Binghamton University
11:00 AM	**Solid-State NMR Mobility Studies of Cellular Prion Protein and Amyloid-β Oligomers.** Lauren Klein, Yale University
11:20 AM	**MAS NMR on Dynamic Domains of Amyloid Fibrils.** Ansgar Siemer, University of Southern California
11:40 AM	**NMR Crystallography in Tryptophan Synthase: Proton Positions, Stable Intermediates, and Transition States.** Leonard Mueller, University of California, Riverside
12.10 PM	Closing remarks and 2020 Vaughan Lecturer Call for Nominations