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** | |
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| 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

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| **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**

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| 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

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| **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<br>*(Enjoy an evening of comradeship, fine food and recognition of peers. Pre-registration required.)* |
| 8:00 PM | **Welcoming Remarks.** Kurt Zilm, Conference Chair |
| 8:05 PM | ***A Half Century of RF, µw's and the Magic Angle*.** Robert G. Griffin, Massachusetts Institute of Technology |
| 8:35 PM | EPR Awards |
| 8:45 PM | SSNMR Awards |

**THURSDAY, JULY 26, 2018**

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| **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 |