

**59th Rocky Mountain Conference on Magnetic Resonance
Solid-state NMR Symposium
Poster Presentations**

Monday, July 23: 7:30-9:30 pm (Authors Present for Posters Labeled A)

Tuesday, July 24: 7:30-9:30 pm (Authors Present for Posters Labeled B)

Late Breaking Additions

A	Optimized Excitation and Refocusing Pulses for the Acquisition of Ultra-Wideline NMR Spectra. <u>Adam R. Altenhof</u> , University of Windsor
B	New ¹H-¹⁴N Indirect Robust Detection Methods that are Either More Efficient or More Resolved. <u>Jean-Paul Amoureux</u> , Lille University
A	Exploring the Hydration of the Inner Earth: Multinuclear NMR Spectroscopy and Ab Initio Random Structure Searching. <u>Sharon E. Ashbrook</u> , University of St Andrews
B	Probing Ion Mobility in Lithium-Rich Anti-Perovskites using Solid-State NMR. <u>Tavleen S. Attari</u> , Durham University
A	²⁰⁷Pb NMR of Ferroelectric Perovskite Lead Germanate at the Paraelectric to Ferroelectric Phase Transition. <u>Claudia E. Avalos</u> , Ecole Polytechnique Fédérale de Lausanne
B	Proton Detection and Dynamics in Ab₁₋₄₂ Fibrils. <u>Salima Bahri</u> , Massachusetts Institute of Technology
A	Nitric Oxide Adsorption in Two Types of Metal-Organic Frameworks (MOFs) - Chemisorption as NONOates Besides Physisorption. <u>Marko Bertmer</u> , Leipzig University
B	Slow Recovery of longitudinal Polarization in the Gas-phase NMR Spectra of Matrix-isolated Molecules. <u>Seth Blackwell</u> , University of Nebraska-Lincoln
A	Status of the Cosmic Axion Spin Precession Experiment (CASPER). <u>John W. Blanchard</u> , Helmholtz-Institut Mainz
B	Towards Nuclear Hyperpolarisation in MOFs. <u>Richard W. Bounds</u> , University of California Berkeley
A	Phase Separation in Silicate Glasses Revealed Through Inverse Laplace Analysis of ²⁹Si T₂ Relaxation. <u>Mark Bovee</u> , The Ohio State University
B	Investigating the Hydrate Forms and Functional Properties of Magnesium Stearate in Pharmaceutical Formulations using Solid-State NMR Spectroscopy. <u>Julie L. Calahan</u> , University of Kentucky
A	Fast MAS Proton Detected ¹⁷O Solid-State NMR Spectroscopy for Enhanced Resolution and Measurement of Scalar and Dipolar Couplings. <u>Scott L. Carnahan</u> , Iowa State University

B	Solid-state NMR of Huntingtin Fibrils. Bethany G. Caulkins, University of Southern California
A	Solid-State NMR Study of Adsorbed Aqueous Salt Solutions in Porous Carbons. L. Cervini, Lancaster University
B	Probing Non-covalent Recognition of Substrates on Silicate Surfaces with DNP-SENS. Kevin R. Chalek, University of California Riverside
A	A Cautionary Tale in Solid-state NMR: Unexpected Bicarbonate Found in Solid Amine Adsorbents for Carbon Capture. Chia-Hsin Chen, Washington University in St. Louis
B	Characterization of Emerging Semiconductor Materials Using Solid-State NMR Spectroscopy. Yunhua Chen, Iowa State University
A	NMR Crystallography: Refinement of Multiple Proton Positions in Hydrated Magnesium Carbonate through $^{13}\text{C}\{^1\text{H}\}$ REDOR and Density Functional Theory Calculation. Jinlei Cui, Washington University in St. Louis
B	Solid State NMR Characterization of NO-releasing Biomedical Tubing. Justin T. Douglas, University of Kansas
A	Comparison of Selectivity and Efficiency of ^1H-^1H Polarization Transfer Between Different Recoupling Sequences Under Ultra-fast MAS. Nghia Tuan Duong, RIKEN-JEOL Collaboration Center
B	Multiple-Quantum Filtered NMR of Sodium Ions in Nafion: Toward Defining the Distribution of Channel Directors. M.A. Eastman, Oklahoma State University
A	Use and Misuse of Scalar J-Couplings in Disordered Inorganic Solids. P. Florian, CEMHTI-CNRS
B	Phase-specific Proton Dynamics in Doped SnP_2O_7 Proton Conductors. Gabrielle Foran, McMaster University
A	Structure and Dynamics in New Materials for CO_2 Capture. Alexander C. Forse, University of California Berkeley
B	Development of Alternative Na-Air Cathodes Using Solid State NMR Spectroscopy. Christopher J Franko, McMaster University
A	The Duet of Acetate and Water at the Defects of Metal-organic Framework. Yao Fu, Zhejiang University
B	DNP SENS of Highly Reactive Heterogeneous Catalysts. David Gajan, Université de Lyon
A	Molecular Structure of Glucagon Fibrils Characterized by Solid-State NMR. Martin D. Gelenter, Massachusetts Institute of Technology
B	A Better Route to Mixed-Linker Cadmium Imidazolate Frameworks. Jacqueline E. Gemus, University of Windsor
A	Cross-Seeding of Mammalian Y145Stop Prion Protein Amyloids Studied by Solid State NMR. Tara George, The Ohio State University
B	Understanding Local Structure and Oxide-ion Dynamics in Functional Paramagnetic Oxides using ^{17}O Solid-state NMR. David M. Halat, University of Cambridge

A	Characterizing the Surface of Nanoparticles with Fast MAS and DNP-Enhanced Solid-State NMR Spectroscopy. Michael P. Hanrahan, Iowa State University
B	Multinuclear Solid-state NMR Studies of Li-Stuffed Garnet-Type Solid Electrolytes. Abby R. Haworth, Durham University
A	Predicting Chemical Shifts of Molecular Crystals using Machine Learning. Albert Hofstetter, Ecole Polytechnique Fédérale de Lausanne
B	Investigating Disorder and Dynamics in a Novel Gallophosphate. Joseph E. Hooper, University of St Andrews
A	Solid-State Dipolar Recoupling NMR Reveals Evidence for Self-Assembly-Driven <i>Trans-to-Cis</i> Amide Bond Isomerization in Peptoid Nanosheets. Benjamin C. Hudson, Georgia Institute of Technology
B	Understanding Battery Cathode Materials Using Solid-State NMR Techniques. Chelsey L. Hurst, McMaster University
A	DFT Spectral Peak Assignments Based on Chemical Shift Anisotropy. Robbie J. Iulucci, Washington and Jefferson College
B	Cluster Formation of Network-Modifier Cations in Cesium Silicate Glasses Studied with ²⁹Si MAF NMR. Daniel Jardón-Álvarez, The Ohio State University
A	Monte Carlo Simulations of NMR Data Acquisition and Processing: Implications for Non-Uniform Sampling. Manpreet Kaler, University of California Riverside
B	Coordination Changes of Trace Elements in High-Pressure Silicate Melts. Nasima Kanwal, University of St Andrews
A	Exposing Halide-Mixing in Hybrid Perovskite Materials using Solid-State NMR. Abhoy Karmakar, University of Alberta
B	Probing the Local Structure of Copper Complexes Through DFT Calculations of Paramagnetic NMR Parameters. Zhipeng Ke, University of St Andrews
A	Instrumentation and Methods Development for NMR of Oriented Biomolecules. John E. Kelly, University of California Irvine
B	Design of a Triple-Resonance Switched Angle Spinning ssNMR Probe for Studies on Protein-Membrane Dynamics. J.I. Kelz, University of California Irvine
A	Sensitivity Enhanced Multi-Quantum MAS NMR Spectroscopy for Spin-3/2 Nuclei Using WURST Amplitude-Shaped Pulses. Robert Knitsch, University of Muenster
B	A General Evaluation of WURST Parameters for Optimized WURST-CPMG Experiments. J. Koppe, University of Münster
A	Multinuclear Solid-State NMR Studies of Si-γ-Al₂O₃ Materials. Bonifác Légrády, University of St Andrews
B	^{121/123}Sb NQR and ¹³C SSNMR Spectroscopic Study of Non-Covalent Pnictogen Bonds. C. Leroy, University of Ottawa
A	The Block Fourier Transform of Non-Uniformly Sampled Time-Domain Signals. Corbin R. Lewis, University of California Riverside

B	NMR Crystallography: Preferred Protonated Positions in α-Aminoacrylate Intermediate. <u>Viktorria Liu</u> , University of California Riverside
A	Probing Volatile Organic Compounds Adsorption Properties on Biomass-based Activated Carbon by ^1H NMR Spectroscopy. <u>Haiyan Mao</u> , University of California Berkeley
B	Insertion of An^{3+} in $(\text{La})\text{PO}_4$ Matrices a Comparison with Rare-earth Surrogates. <u>L. Martel</u> , European Commission
A	Magnetization, Specific Heat, ^{17}O NMR and ^{237}Np Mössbauer Study of $\text{U}_{0.15}\text{Np}_{0.85}\text{O}_2$. <u>L. Martel</u> , European Commission
B	Complete Structural Assignment of a Pharmaceutical Drug by Combining DNP-Enhanced Solid-State NMR and DFT Calculations. <u>Renny Mathew</u> , New York University Abu Dhabi
A	Evaluation of Stacking in 2D Covalent Organic Framework by Solid State NMR. <u>Igor Moudrakovski</u> , Max-Planck Institute for Solid State Research
B	Structural Assessment of Titanates with High Field $^{47,49}\text{Ti}$ Solid State NMR and First Principles Calculations. <u>Igor Moudrakovski</u> , Max-Planck Institute for Solid State Research
A	In Situ High-Pressure Solid State NMR Under Magic Angle Spinning. <u>Filipp Mueller</u> , New York University Abu Dhabi
B	Bulk Heterojunction Interfacial Structure from REDOR NMR. <u>R. C. Nieuwendaal</u> , National Institute of Standards and Technology
A	Identification of the Strong Brønsted Acid Site in a Metal-Organic Framework Solid Acid Catalyst. <u>Thomas M. Osborn Popp</u> , University of California Berkeley
B	Investigation of the Li-ion Conduction Behavior in the $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$ Solid Electrolyte by Two-dimensional T_1-spin Alignment Echo Correlation NMR. <u>M.C. Paulus</u> , Forschungszentrum Jülich GmbH
A	Mechanochemical Syntheses and ^{35}Cl Solid-State NMR Characterization of Fluoxetine HCl Cocrystals. <u>A.A. Peach</u> , University of Windsor
B	Investigation of Plant Cell Wall Structure Using ^1H and ^{13}C-Detected Fast MAS Solid-State NMR. <u>Pyae Phy</u> , Massachusetts Institute of Technology
A	Computational Studies of ^{29}Si NMR in Crystalline and Amorphous Silicon Nitrides. <u>Iliia Ponomarev</u> , University of Texas at Arlington
B	Computational Investigations of ^{29}Si and ^{31}P NMR data in Silicophosphates. <u>Iliia Ponomarev</u> , University of Texas at Arlington
A	Solid-state NMR Study of Flexibility in Zeolite Frameworks. <u>Suzi M. Pugh</u> , University of St Andrews
B	Amide Versus Amine Ratio in the Discrimination Layer of Reverse Osmosis Membrane by Solid State ^{15}N NMR and DNP NMR. <u>XiaoHua Qiu</u> , The Dow Chemical Company
A	Solid State NMR Studies of a Rhodium σ-alkane Complex C-H Activation by Solid/Gas Single-Crystal to Single-Crystal H/D Exchange. <u>Nicholas H. Rees</u> , University of Oxford

B	Solid-State NMR Study of Poly(ethylene Oxide) Crystals: The Effect of a Well-Defined Point Defect in the Middle of Polymer Chain. <u>Detlef Reichert</u> , Martin Luther University of Halle-Wittenberg
A	Investigating Breathing Effects in Metal-Organic Frameworks Using Solid-State NMR Spectroscopy. <u>Cameron M. Rice</u> , University of St Andrews
B	Molecular Mobility and Packing in Polyelectrolyte and Hybrid Systems. <u>Ulrich Scheler</u> , Leibniz-Institut für Polymerforschung Dresden e.V.
A	Insights on Acid Site and Defect Site Pairing in Zeolites via Multiple-Quantum ¹H MAS NMR. <u>C. Schroeder</u> , University of Münster
B	Insights into the Solid-State Synthesis and Structures of Zeolitic Imidazolate Framework Materials from NMR-Enhanced Crystallography. <u>R. W. Schurko</u> , University of Windsor
A	Fast Magic Angle Spinning + Dynamic Nuclear Polarization: Better, Faster, Stronger, Narrower. <u>Ivan V. Sergeyev</u> , Bruker Biospin Corporation
B	Historical Review and New Insights into SiAlON Materials. <u>Valerie R. Seymour</u> , Lancaster University
A	A Combined ²⁵Mg Solid-State NMR and DFT Approach to Probe the Local Structural Differences in Magnesium Acetates Mg(CH₃COO)₂·nH₂O (n = 0, 1, 4). <u>Valerie R. Seymour</u> , Lancaster University
B	Rapid Measurement of Long-Range Distances in Proteins by Multidimensional ¹³C-¹⁹F REDOR NMR under Fast Magic-Angle Spinning. <u>Alexander A. Shcherbakov</u> , Massachusetts Institute of Technology
A	Dynamic Nuclear Polarization of Silicon Microparticles. <u>D. Shimon</u> , Dartmouth College
B	⁹³Nb NMR Structural Analysis of Acid-Exchanged Layered Bismuth Niobate Perovskites with Varying Band Gaps. <u>Luis Smith</u> , Clark University
A	Classification of the Number of Attached Protons for ¹⁵N Nuclei in the Solid State. <u>Sarah E. Soss</u> , University of Utah
B	Linear Inversion of Anisotropic NMR Spectra. <u>Deepansh Srivastava</u> , The Ohio State University
A	The Melanization Road More Traveled by: Pigment Development in Cell-free and Fungal Cell Systems. <u>Ruth E. Stark</u> , City University of New York
B	²⁹Si Solid-state NMR Database of Tensors for Crystalline Materials in The Materials Project. <u>He Sun</u> , Washington University in St. Louis
A	Characterization of the Active Phase Formed on Boron Nitride Oxidative Dehydrogenation Catalysts Using MAS NMR and SEM. <u>Brijith Thomas</u> , Iowa State University
B	Lipid Membrane Fusion Mechanism of Pulmonary Surfactant Peptide B₁₋₂₅. <u>N.T. Tran</u> , University of Florida

A	Solution and Solid-State NMR Investigations into the Phase States of Cellular Prion Protein and Amyloid-β Oligomer Complexes. Marcus D. Tuttle, Yale University
B	Solid State NMR Investigation of Mechanically Driven Mineral Carbonation. John S. Vaughn, Lawrence Livermore National Laboratory
A	Proton Detection of Unreceptive and Exotic Nuclei. Amrit Venkatesh, Iowa State University
B	Multinuclear Solid-State NMR Spectroscopy of Ionic Cocrystals. C.S. Vojvodin, University of Windsor
A	Operando MAS-NMR Studies of Mixed Phase Systems at Elevated Temperatures and Pressures. Eric D. Walter, Pacific Northwest National Laboratory
B	Czjzek Lineshape Analysis of Quadrupolar NMR Spectra of Disordered Materials. Sungsool Wi, National High Magnetic Field Laboratory
A	Rapid Characterization of Formulated Pharmaceuticals Using Fast MAS ^1H Solid-State NMR Spectroscopy. Anuradha V Wijesekara, Iowa State University
B	Structural Evaluation of Designer Co-assembling Peptide Nanofibers. Kong M. Wong, Georgia Institute of Technology
A	^{31}P and ^{17}O Single-Crystal NMR Characterization of Halogen-Bonded Cocrystals. Y. Xu, University of Ottawa
B	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