

**61st Rocky Mountain Conference on Magnetic Resonance
Solid-state NMR Symposium
Poster Presentations**

Tuesday, July 26: 7:30-9:30 pm (Authors Present for Posters Labeled A)

Wednesday, July 27: 7:30-9:30 pm (Authors Present for Posters Labeled B)

A	Electron Spin Control in Cryogenic MAS DNP. Nicholas Alaniva, ETH Zürich
B	Positional Uncertainties in NMR Assisted Crystallography of Tryptophan Synthase. David C. Amarasinghe, University of California Riverside
A	Novel Sampling Schemes for the Indirect Detection of Ultrawideline ¹⁹⁵Pt Solid-State NMR Spectra for the Characterization of Heterogeneous Catalysts. Benjamin A. Atterberry, US DOE Ames Laboratory
B	In-Cell Quantification of Drugs by Magic-Angle Spinning Dynamic Nuclear Polarization NMR. Pierrick Berruyer, École Polytechnique Fédérale de Lausanne (EPFL)
A	The Role of Methyl Dynamics in DNP. Thomas Biedenbänder, University of Rostock
B	Using Solid-state NMR Spectroscopy to Investigate Mixed-metal MIL-53. Emma A. L. Borthwick, University of St Andrews
A	NMR Investigations of the Structural Role of Phosphorus in Aluminosilicate Glasses for Ion Exchange. Mark O. Bovee, The Ohio State University
B	Alternative Methods for Generating Endogenous Radicals for High-Field MAS DNP. Scott Carnahan, Ames Laboratory
A	Probing Cation-π Interactions in Spider Silk Fibers with Selective DARR Difference MAS SSNMR. Kevin R. Chalek, San Diego State University
B	Insight into the Curvature Control Mechanism of the Rous Sarcoma Virus Capsid Protein Assembly. Bo Chen, University of Central Florida
A	Teaching Solid-state NMR as Part of a Graduate NMR Course. Catherine F.M. Clewett, University of Wisconsin Madison
B	Structure and Dynamics of Glass-Forming Metal Organic Frameworks. Ieuan Cornu, CNRS
A	Influences of Mechanical Compression on the Molecular ⁷Li Dynamics in Solid Electrolytes (SEs). Mengyang Cui, McMaster University
B	Solid-state NMR Spectroscopy Investigation of Al,Ga-containing Metal-Organic Frameworks. Z. H. Davis, University of St Andrews
A	Remodeling of the Fungal Cell Wall Structure by Antifungal Drug. Malitha C. Dickwella Widanage, Louisiana State University
B	Dynamic Nuclear Polarization Enhanced ¹¹⁹Sn Solid-state NMR Spectroscopy for the Structural Characterization of Tin in Toothpaste. Rick W. Dorn, US DOE Ames Laboratory
A	Showcasing Advanced NMR Approaches to Probe Li Ion Dynamics in Several Crystal Structures. Benjamin B. Duff, University of Liverpool
B	Tailored Biradical for Cross-Effect DNP at High Magnetic Field and Fast MAS. Asif Eqbal, University of California Santa Barbara
A	Determining the Internal Orientation of Elongated Nanocavities by NMR. Gregory Furman, Ben Gurion University of the Negev
B	Three-Dimensional Structure Determination of a Supported Molecular Catalyst with Multiple Surface Sites. David Gajan, Université de Lyon
A	MAS Spherical Shell Rotors and Spherical Solenoid Coils Boost RF Homogeneity and NMR Sensitivity. Chukun Gao, ETH Zürich

B	Investigating conformational Ensemble of Alzheimer's Disease Protein, Tau using Dynamic Nuclear Polarization SSNMR. Rupam Ghosh, UT Southwestern Medical Center
A	<i>mrsimulator</i>: A Cross-Platform, Object-Oriented, and Open-Source Software Package for Fast Solid-state NMR Spectral Simulation and Analysis. M. D. Giammar, The Ohio State University
B	Unraveling Structure-property Relationships in Carbonaceous Materials Obtained via Methane Pyrolysis using Solid-state NMR, XPS, and Electrochemical Characterization. Raynald Giovine, University of California Santa Barbara
A	Electrochemical Complexation of Polyatomic Aluminum Ions to Heterogeneous Organic Electrode Samples Investigated Using Solid-state Dipolar-mediated NMR Methods. Leo W. Gordon, City College of New York
B	Study of Methyl Rotations in Halogen Bonded Cocrystals via Deuterium NMR Using T₁ Time Constants. Shubha S. Gunaga, University of Ottawa
A	Massive C_Q's and Fast Cation Dynamics: ²³Na, ²⁵Mg and ¹¹B NMR Studies of "Paddlewheel" Antiperovskite Solid Electrolytes. David M. Halat, Lawrence Berkeley National Laboratory
B	Electrophoretic NMR Reveals Migration of Solvation Structures in Li-ion Battery Electrolytes. David M. Halat, Lawrence Berkeley National Laboratory
A	Understanding the Mechanochemical Synthesis of [Cu(Cl)(NHC)] Complexes using Solid-state NMR Spectroscopy. Lama Hamdouna, Université de Lille
B	Solid-state NMR ¹³C Sensitivity at High Magnetic Field. Ruixian Han, University of Wisconsin Madison
A	Do NMR Crystallography Structural Relaxations Matter? James K. Harper, Brigham Young University
B	A Software Tool for Refining Crystal Structures using ¹³C NMR Chemical Shift Tensors as a Target Function. James K. Harper, Brigham Young University
A	Improving the Accuracy of GIPAW Chemical Shielding Calculations with Cluster and Fragment Corrections. Joshua D. Hartman, Mt. San Jacinto College
B	Understanding the Local Structure of Protective Alumina Coatings for Cathodes and the Coating-Cathode Interface. Abby R. Haworth, Lancaster University
A	NMR-assisted Crystallography Reveals Hydrogen Atom Positions and Reduced Positional Uncertainties for the Tryptophan Synthase Aminoacrylate Intermediate. Jacob Holmes, University of California Riverside
B	Toward Determining the Structures of Human γS-crystallin in the Native and Aggregated States using Bicelles and Solid-state NMR. Matthew Jimenez, University of California Irvine
A	Characterization of Gaseous CO₂-Amine Reactions in Solid Amine Sorbents with Nuclear Magnetic Resonance. Patrick T. Judge, Washington University in St. Louis
B	Solid-state and <i>in situ</i> NMR Insights into the Role of Metal-organic Frameworks in Moderating Pt-based Catalysts for Alcohol Electrooxidation. Arafat Hossain Khan, TU Dresden
A	Assignment of the Highly Disorder Reflectin (Ref2C)₄: A Protein from the Skin of Squid. Md Imran Khan, University of Central Florida
B	The Periodic Table Opens Further: New Insights into Broadband Cross Polarization to Half-Integer Quadrupolar Nuclei. James J. Kimball, Florida State University
A	High Resolution Solid-state NMR in Paramagnetic Metal-Organic Frameworks. C.A. Klug, U.S. Naval Research Laboratory
B	DNP-Enhanced Solid-state NMR with a Polarization Transforming Reflector. Guillaume P. Laurent, US DOE Ames Laboratory
A	Integrated Software Technologies for Biomolecular Solid-state NMR. Woonghee Lee, University of Colorado Denver

B	NMR Study of Aqueous Electrolyte Adsorption in Porous Carbon. Dongxun Lyu, University of Cambridge
A	Diffusion Mechanisms of DNA in Agarose Gels – NMR Studies and Monte Carlo Simulations. Günter Majer, Max Planck Institute for Intelligent Systems
B	Understanding Interactions Between Resistant Microbes and Drug Loaded Colloidal Nanomaterials using ‘On Cell’ NMR Spectroscopy. Katarzyna Malec, Wroclaw Medical University
A	Scalable Nanoporous Networks for CO₂ Chemisorption via Solid-state NMR Spectroscopy. Haiyan Mao, University of California Berkeley
B	Modeling and Optimization of Multiple-Quantum Magic-Angle Spinning NMR Spectra. Lexi McCarthy, The Ohio State University
A	Probing Solid Solutions and Cocrystals in Pharmaceutical Compounds using Solid-state NMR. Jiashan Mi, Iowa State University
B	A ⁵⁵Mn ssNMR Investigation of Manganese Dioxide 1x2 Tunnel Polymorphs. Anne Mirich, University of Connecticut
A	NMR Methods for Hybrid Perovskites. Aditya Mishra, École Polytechnique Fédérale de Lausanne (EPFL)
B	Optimum Signal-to-Noise in Non-Uniform Weighted Sampling. Leonard J. Mueller, University of California Riverside
A	⁷⁷Se and ¹²⁵Te Solid-State NMR and X-ray Diffraction Study of Chalcogen-Bonded 3,4-Dicyano-1,2,5-Chalcogenodiazole Cocrystals. Tamali Nag, University of Ottawa
B	The Magnetic Properties of MAI₄(OH)₁₂SO₄·3H₂O with M = Co²⁺, Ni²⁺, and Cu²⁺ - a New Class of Lowdimensional Spin Systems. Ulla Gro Nielsen, University of Southern Denmark
A	Correlation and Distance Measurements Between ¹H and ¹⁴N using ¹⁴N Overtone NMR Spectroscopy. Yusuke Nishiyama, RIKEN
B	Single Crystal Sapphire as an <i>in situ</i> Angle Sensor for MAS NMR. Thomas M. Osborn Popp, Rutgers University
A	Studies of Lithium-ion Dynamics and Structural Changes in LiFeV₂O₇ by Solid-state NMR. Taiana L. E. Pereira, McMaster University
B	Determination of Accurate ¹⁹F Chemical Shift Tensors with R-Symmetry Recoupling at High MAS Frequencies (60-100 kHz). Gal Porat-Dahlerbruch, University of Delaware
A	ssNMR Investigation on Disorder Novel Semiconducting Material AAe₆Si₁₂P₂₀X (A = Na, K, Rb, Cs; Ae = Sr, Ba; X = Cl, I, Br). Andrew P. Porter, Iowa State University
B	DNP using Spherical Rotors. Lauren Price, ETH Zürich
A	Integrated, Stretched and Adiabatic Solid Effects. Yifan Quan, Massachusetts Institute of Technology
B	¹⁷O NMR Reveals CO₂ Capture Mechanisms in Hydroxide-functionalised Metal-organic Frameworks. Benjamin J. Rhodes, University of Cambridge
A	Molecular-level Effects of Radiation and Electrochemical Discharge on Li-CF_x Batteries for Space Exploration. Loleth E. Robinson, City College of New York
B	Comparing Methyl Groups Dynamics in the Hydrophobic Core of Amyloid-beta (1-40) Fibrils by ²H Solid-state NMR Line Shape Analysis: In the Wild-type Form, Serine-8 Post-translational Modification, and the Cross-seeded Variant. Aryana Rodgers, University of Colorado at Denver
A	¹H{³⁵Cl} and ²⁹Si{³⁵Cl} RESPDOR Solid-State NMR Spectroscopy Experiments Reveal Chlorine Functionalization of 2D Silicane Sheets. Aaron J. Rossini, Ames Laboratory
B	Development of ¹⁹F Fast Magic-Angle-Spinning NMR Spectroscopy for Protein Structure Determination using Crystalline Lectin Oscillatoria Agardhii Agglutinin. Brent R. Runge, University of Delaware
A	Charge Compensation, Hydrogen Bonds and Packing of Polyanions in Polyelectrolyte Complexes. Ulrich Scheler, Leibniz-Institut für Polymerforschung Dresden e.V.

B	Ultra-High Field ^{103}Rh Solid-state NMR: New Experimental and Theoretical Pathways. Jasmin Schoenart, Florida State University
A	Developing Methods for the Acidity Measurements on Supported Ni Catalysts. Mirjam Schröder, University of Rostock
B	Microwave Reflection and Absorption under High Field MAS-DNP Conditions for Probe Building. Faith J. Scott, National High Magnetic Field Laboratory
A	Combining Solid-state NMR with DEER EPR to Study Structure and Dynamics of Cross-β Fibrils. Ansgar Siemer, University of Southern California
B	PIETA Based Pathway Selection of Non-frequency Dispersed Echoes in WURST-CPMG. Luis Smith, Clark University
A	^{67}Zn, ^{27}Al, and ^{71}Ga Solid-state NMR of Zinc Oxide Nanoparticles. Robert B. Smith, Florida State University
B	Understanding Diffusion Properties in Metal Organic Frameworks/Polymer Composites for CO_2 Capture by NMR Studies. Ah-Young Song, Lawrence Berkeley National Laboratory
A	Is ^1H CSA Useful for the Measurement of Dynamics in Heterogeneous Catalysts? Scott A. Southern, US DOE Ames Laboratory
B	Nuclear Magnetic Ordering in Naphthalene. Jakob M. Steiner, Paul Scherrer Institut
A	^{27}Al NMR Chemical Shielding and Quadrupolar Tensors Benchmarking with DFT: Machine Learning Prediction of Quadrupolar Coupling Constants (C_Q) from Simple Local Geometry and Elemental Properties. He Sun, Washington University in St. Louis
B	Materials Innovation for Carbon Capture by Advanced Magnetic Resonance Methods. Jing Tang, Stanford University
A	Distinct Pore-forming Conformation of Amyloid Beta Peptide $\text{A}\beta_{1-42}$ in Membrane Environments. Tyrone Thames, University of Central Florida
B	Rapid Protein Secondary Structure Determination from a Single Unassigned 1D ^{13}C NMR Spectrum. Marcus Tuttle, Yale University
A	Developments in Automation and Additive Manufacturing Techniques in the ssNMR Maker Space. Jose L. Uribe, University of California Irvine
B	NMR Crystallography of Organic Anode Materials for Lithium- and Sodium-ion Batteries. Tommy Whewell, Lancaster University
A	Uncovering Sequence-Structure Relationships for Engineering Coassembled Peptide Nanofibers. Kong M. Wong, Georgia Institute of Technology
B	Probing Allosteric Coupling and Allosteric Participants in a Potassium Channel by SSNMR. Yunyao Xu, Columbia University
A	Determination of Histidine Protonation States in Proteins by Fast Magic Angle Spinning NMR. Roman Zadorozhnyi, University of Delaware
B	Application of Solid-state NMR Spectroscopy in Pharmaceutical Research and Development. Siwei Zhang, AbbVie Inc.
A	Investigation of Cooperative CO_2 Capture in Amine-Functionalized Metal–Organic Frameworks (MOFs) by Solid-state NMR. Hao Zhuang, University of California Berkeley