Event Agenda

PANIC and MANIC 2026

Monday, May 04, 2026

Breakfast (provided by PANIC)

8:00 AM – 9:00 AM

PANIC

Don't PANIC Tutorial

9:00 AM – 9:30 AM

PANIC

Speaker

Louis Madsen

Professor | Virginia Tech

> ### Introduction to polymer NMR – How to assess your sample and start some useful experiments
>
> 9:00 AM – 9:30 AM
>
> PANIC
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> So you're a well-trained NMR spectroscopist… Where do you start if someone asks you to analyze a gel, or a polymer electrolyte membrane, or nanoparticles in suspension, or a polymeric micelle solution? Do you need to do magic-angle spinning experiments, or under what conditions will your solution probe work? How much sample do you need and how should you formulate it? How will your spectrum change with your sample's composition/concentration? Does your sample contain more than one material or phase? When and how do you need to modify your acquisition parameters? What nuclei might be most "friendly" and why? These types of questions can put you rather far away from the normal space of biochemical and organic chemical NMR spectroscopy. In this tutorial talk, I will provide strategies and rules of thumb for some typical situations when trying to understand polymer solutions and polymer-based materials. A key example: Often your spectral information changes drastically with polymer content, so it can help to incorporate a very informative "indirect dimension" into your NMR experiment by systematically collecting spectra as a function of polymer weight %.
>
> **Speaker**
>
> 
>
> **Louis Madsen**
>
> Professor | Virginia Tech

JEOL User Meeting

9:30 AM – 11:30 AM

PANIC

Don't PANIC Tutorial

11:30 AM – 12:00 PM

PANIC

Speaker

Subrata Mishra

Principal Investigator | NIST

Water, Water Everywhere: Making It Disappear (Properly)

11:30 AM – 12:00 PM

PANIC

Water is the solvent of choice for many NMR experiments — and often the source of much frustration when not dealt with properly. In aqueous samples, its intense resonance can overwhelm receiver dynamic range, distort baselines, promote radiation damping, and mask exchangeable signals. This workshop introduces a framework for understanding how different water suppression strategies work and when they fail. The session will outline decision criteria for selecting an appropriate strategy based on your experimental goals. Attendees will leave with practical guidance for optimizing solvent suppression in real-world aqueous NMR experiments.

Speaker

Subrata Mishra

Principal Investigator | NIST

Lunch (provided by PANIC)

12:00 PM – 1:00 PM

PANIC

Bruker User Meeting

1:00 PM – 3:00 PM

PANIC

Don't PANIC Tutorial

3:00 PM – 3:30 PM

PANIC

Speaker

Ryan Nieuwendaal

Research Physical Chemist | National Institute of Standards and Technology

What makes the magic angle so magical? - A brief introduction to solid-state NMR

3:00 PM – 3:30 PM

PANIC

Spinning solids at the magic angle is a central feature of all solid-state NMR research. However, have you ever stopped to think "What makes that one angle, 54.7°, so magical?" In this tutorial, I will walk through the fundamentals of magic angle spinning, why you can acquire liquid-like NMR spectra on solid-state samples, and how you can be rest assured that it will work every time. I'll also discuss some of aspects and applications of magic angle spinning that are important for determining internuclear distances, torsion angles, and domain sizes; all key features that set solid-state NMR apart from other analytical techniques.

Speaker

Ryan Nieuwendaal

Research Physical Chemist | National Institute of Standards and Technology

Coffee Break

3:30 PM – 4:00 PM

PANIC

SciY User Meeting

4:00 PM – 6:00 PM

PANIC

Don't PANIC Tutorial

6:00 PM – 6:30 PM

PANIC

Speaker

Matthew Augustine

Professor | UC Davis

> ### Time Domain NMR
>
> 6:00 PM – 6:30 PM
>
> PANIC
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> This tutorial lecture begins by answering the question, “What is time domain NMR ?” Following this definition additional basic questions will be addressed like “What is measured ?”, “How is it measured ?”, and “what does it mean ?”. Within this structure, parameters like T_1, T_2 and D will be explained, the equipment and pulse sequences needed to experimentally obtain these constants will be described, and the treatment of time domain data with non-linear least squares, inverse Laplace transforms and other methods will be surveyed. Recent laboratory and factory examples of time domain of time domain NMR will also be included.
>
> **Speaker**
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> 
>
> **Matthew Augustine**
>
> Professor | UC Davis

Opening Reception (sponsored by SP-Wilmad)

6:30 PM – 8:00 PM

PANIC

Opening reception sponsored by SP-Wilmad with interactive product showcasing and complimentary snacks and drinks.

Tuesday, May 05, 2026

Breakfast (provided by PANIC)

7:45 AM – 8:45 AM

PANIC

Opening Remarks

8:45 AM – 8:55 AM

PANIC

From Peaks to Patients: NMR in Pharma

8:55 AM – 10:30 AM

PANIC

Session Chair: Samantha Miller, Subrata Mishra

Speakers

Haihong Wu

Principal Scientist I | AbbVie

Elodie Crublet

CEO | NMR-BIO

Ciaran Lynch

Associate Principal Scientist, Analytical Research & Development | Merck & Co. Inc.

Protein-Based NMR Applications in Early Drug Discovery

9:00 AM – 9:30 AM

PANIC

Protein-based nuclear magnetic resonance (NMR) is a versatile and powerful tool for early-stage drug discovery, offering atomic-level insights into protein-ligand interactions across a broad affinity range. NMR enables clear confirmation of screening hits and drug leads, minimizing false positives. While conventional protein-detect NMR relies on isotopic labeling of proteins, recent innovations such as 1D-diffusion filters and ECHOS analysis now allow affinity measurements with unlabeled proteins, expanding its utility across more targets. This talk highlights how protein-detect NMR workflows are integrated into our lead discovery pipelines involving various screening modalities such as DNA-encoded libraries (DEL), high-throughput screening (HTS), virtual library screening (VLS), and fragment-based drug design (FBDD).

Speaker

H

Haihong Wu

Principal Scientist I | AbbVie

A New Route to Antibody methyl NMR for Resonance Assignment and HOS Analysis

9:30 AM – 10:00 AM

PANIC

Monoclonal antibodies (mAbs) are critical therapeutic agents whose efficacy rely on the integrity of their higher-order structure (HOS). Subtle HOS perturbations caused by chemical degradation, formulation changes or storage conditions may impair antigen binding. NMR spectroscopy, particularly methyl-NMR, provides atomic-resolution insight into such changes using conventional ^{13}C natural-abundance spectra, but its application to antibodies is limited by low sensitivity and difficulties in resonance assignment.
Here, we present a collaborative project between NMR-Bio, Sanofi and the *Institut de Biologie Structurale* aimed at overcoming these limitations. We describe an optimized strategy for site-specific ^{13}CH$_3$ labeling of antibodies expressed in mammalian CHO cells, combining regio- and stereoselective synthesis of isoleucine and valine methyl precursors with partial deuteration and tailored incorporation protocols. Applied to an anti-LAMP1 antibody, this approach yields highly resolved methyl NMR spectra, enables transfer of Fab and Fc assignments and allows assignment of ~84% of methyl resonances in the intact mAb.
This strategy enables detailed characterization of folding and stability in fully glycosylated antibodies. By overcoming longstanding limitations in labeling efficiency and spectral quality, this approach opens new avenues for atomic-level investigations of large, complex biologics and delivers transformative insights into antibody structure and function.

Speaker

Elodie Crublet

CEO | NMR-BIO

Building a Benchtop NMR Toolbox for Measuring Multiple Attributes in Formulated Biologics

10:00 AM – 10:30 AM

PANIC

Given the rapidly growing diversity of biologic modalities in pharmaceutical pipelines, there is a need for analytical techniques that can rapidly and accurately measure multiple critical quality attributes (CQAs) in formulated biologic drug substance (DS). CQAs such as excipient concentration and pH are traditionally measured using liquid chromatography (LC), mass spectrometry (MS), and conventional pH probes. LC-based methods for excipient quantification, such as UPLC-CAD, the “gold standard” for non-ionic surfactant (NISE) analysis, are laborious, error-prone, non-linear, and destructive, as active biological material is discarded. Traditional pH meters require frequent calibration, suffer from reproducibility issues, and are invasive, potentially affecting sample integrity. To address these limitations, we evaluated low-field NMR as a non-destructive, more user-friendly alternative for quantifying surfactants/other excipients and measuring pH in formulated biologic DS. Our results show that benchtop qNMR provides a fit-for-purpose, reliable, user-friendly, and green route to quantify NISEs and other excipients. Furthermore, benchtop 1H NMR enables accurate, precise, and non-invasive pH measurements, allowing multiple CQAs to be monitored in a single measurement and positioning low-field NMR for routine use in analytical and QC laboratories.

Speaker

Ciaran Lynch

Associate Principal Scientist, Analytical Research & Development | Merck & Co. Inc.

Coffee Break

10:30 AM – 10:55 AM

PANIC

UncommoNMR

10:55 AM – 1:00 PM

PANIC

This session will explore NMR applications that are not widely discussed. We will hear about the role that NMR spectroscopy plays in settings like museums, battlefields, and drug detection.

Session Chairs: Savanah Shumaker, Gennady Khirich

Speakers

Alexander Marchione

Principal Chemist | Chemours

Margaret MacDonald

Research Chemist | US Army DEVCOM Chemical Biological Center

Nick Cutmore

CTO | MagnaTerra

Matthew Augustine

Professor | UC Davis

NMR Experiments in the Gas Phase

11:00 AM – 11:30 AM

PANIC

NMR experiments in the gas phase, though rarely practiced, are a uniquely informative tool for qualitative and quantitative assays, in situ reaction kinetics, and physiochemical studies (e.g. vapor pressure, gas-liquid partitioning). The major practical difference in the spin physics of gaseous systems near ambient pressure is the prevalence of the spin-rotation relaxation mechanism in certain nuclei (esp. ^{19}F and ^{13}C). With these nuclei, the loss in resolution from accelerated spin-spin relaxation is concomitant with acceleration of spin-lattice relaxation, increasing effective sensitivity of the experiment. For identification of unknown analytes in the gas phase, many standard scalar-coupling based correlation experiments can be applied, as well as high resolution diffusion (DOSY) experiments. Homogeneous and heterogeneous gas phase reactions can be studied conveniently in glassware near ambient pressure, and in specialized cells at higher pressure. Finally, gas phase NMR provides perhaps the most convenient means to determine speciated vapor pressure or gas-liquid partitioning constants. Examples of all these experiments will be presented.

Speaker

Alexander Marchione

Principal Chemist | Chemours

Practical Application of NMR Spectroscopy for the Battlefield and in the Museum

11:30 AM – 12:00 PM

PANIC

NMR spectroscopy can be utilized in the lab to resolve practical challenges in themuseum and the battlefield. For example, the development and use of non-invasive analytical tools to explore the surface and subsurface of whole/unmodified porous materials such as hydrogels, paint films, paper-based materials, stone objects, textiles, rubber, and plastics, is of critical importance to both the DOD and the Cultural Heritage field. Through depth profiling and spatially resolved T_2 relaxation experiments, the portable NMR-MOUSE spectrometer observes if a liquid remains on the surface or enters the material, where it is spatially located, if it is restricted within the pore or bound to the surface of pore, and if it evaporates from or persists within the material. One application undertaken in collaboration with University of Maryland Baltimore County SCIART program,involved probing the efficacy of an ion-exchange resin/hydrogel conservation desalination technique for Egyptian limestone relevant to objects found in The Walters Art Museum. NMR spectroscopy has also been utilized in the lab to resolve practical challenges relevant to the warfighter. Questions such as what is the rate of hydrolysis of a threat compound in drinking water, at different pHs, with a variety of caustic solutions, within a porous material like concrete? These bench-top NMR experiments enable decision-making for the warfighter and the conservator, both.

Speaker

Margaret MacDonald

Research Chemist | US Army DEVCOM Chemical Biological Center

Novel NQR systems for the field detection of explosives and drugs

12:00 PM – 12:30 PM

PANIC

Nuclear quadrupole resonance (NQR) based detection has been the focus of many developments due to the promise of precise stand-off analysis without the burden of a magnet, which makes engineered systems more field portable. However, the exceptionally weak response, combined with radio frequency interference in the MHz bands has often limited their usefulness.

NQR developments by CSIRO (Australia's National Science Agency) over two decades have mitigated the impact of radio frequency interference, temperature drift and sensor design on measurement, and rugged field worthy systems have been developed for real time field analysis. MagnaTerra Limited is commercialising this technology for applications in the detection of minerals, explosives and drugs

The development of a handheld NQR system for humanitarian demining is a priority. Over 60 countries are impacted by landmines, and they experience ~8000 casualties per year. Existing methods, relying on metal detection and object shape recognition (radar), are confused by false detections that make landmine removal a very slow, and often, dangerous process. The direct detection of explosives using NQR can significantly speed landmine detection and subsequent land release to local communities.

The development of an NQR based handheld landmine detector and its trial in Angolan minefields is described, and the continuing developments required for wider global applications in demining are explained.

Speaker

N

Nick Cutmore

CTO | MagnaTerra

Free Resolution in Liquids and Increased Signal in Solids Benchtop NMR

12:30 PM – 1:00 PM

PANIC

Speaker

Matthew Augustine

Professor | UC Davis

Lunch (provided by PANIC)

1:00 PM – 2:00 PM

PANIC

Posters - Session 1 (even-numbered) including Coffee Break

2:00 PM – 3:55 PM

PANIC

Poster 2: Quality Control Assays of Polyurethane Raw Materials Using Benchtop NMR Spectroscopy (Susie Riegel)

Poster 4: Quantitative Diffusion for Macromolecules in Complex Mixtures with Benchtop NMR (Blake Fonda)

Poster 6: Resolving Catecholamine–Membrane Interactions in Complex Lipid Environments (Emmanuel Osei)

Poster 8: Synthesis and Characterization of New Isomeric Pt-Doped Au_{25} Alloy Molecular Nanoclusters (Terfa Igba)

Poster 10: NMR Informed Mixture Identification System (NIMIS): A Chemically Informed Slot-Attention Framework for Demixing 1D-^{1}H-NMR Mixture Spectra (Anna Marija Sumrova)

Poster 12: Investigating a purported connection between DNO and Mass (Mark Sokol)

Poster 14: Resolving ambiguities in NMR assignments of small molecules (Claire Dickson)

Poster 16: A Cell-Based NMR Platform for the Characterization of Drug-Receptor Interactions (Christopher Williams)

Poster 18: 19F NMR in the identification and quantification of fluorotelomer alcohols in food packaging materials (Jennifer Janovick)

Poster 20: Probing molecular exchange in functional materials using variable-temperature 1D NMR and line shape analysis (Shravan Uppala)

Poster 22: Analysis of PFAS content of clam and deer meat samples using 19F NMR in combination with LC/HR-MS (Clark Ridge)

Poster 24: Characterizing non-equilibrium self-assembly dynamics of supramolecular polymers using cryo-synchronized reactions (Tianyue Dai)

Poster 26: Solvent-Dependent Conformational Analysis of Ipglycermide Cyclic Peptides by NMR (Samuel Kotler)

Poster 28: Transport and Morphology in Molecular Ionic Composite Electrolytes via NMR Diffusometry and Relaxometry (Nicholas Pietra)

Poster 30: NMR of Confined [BMIM][TCM] in Mesoporous Silica: Relevance to Biomass-Derived Carbon (Jamal Hassan)

Poster 32: Enhancing oligonucleotide therapeutic characterization through bioanalytical techniques and computational modeling (Akanksha Manghrani)

SMASH at PANIC

3:55 PM – 5:30 PM

PANIC

SMASH is dedicated to recognizing scientific contributions that further our knowledge and understanding of small molecules through the lens of NMR spectroscopy. The collaboration between SMASH and PANIC strengthens the global NMR community by creating shared forums for scientific discussion and exchange. This year presentations will focus on new applications to decipher the mechanism behind a light-based cancer treatment, a new computational approach to unravel the complex conformational behavior of macrocyclic peptides, and the journey of an NMR spectroscopist supporting the development of new investigational drugs from discovery to market.

Session Chair: Clark Ridge

Speakers

Thomas Williamson

Distinguished Professor | University of North Carolina Wilmington

Alexei Buevich

Principal Scientist | Merck and Co., Inc.

Kathleen Farley

Senior Consultant | Solution NMR Analytics LLC

Investigation of Light-Induced Therapeutic Effects of Inorganic Ru(II) Complexes Using LED-NMR

4:00 PM – 4:30 PM

PANIC

Ru(II) polypyridyl systems have become ideal photosensitizing agents in photodynamic therapy, as they offer DNA-binding properties, display photoluminescence, and exhibit tunable photophysical and electrochemical properties. Researchers are developing Ru(II) complexes to engage in a similar mechanism of action to cisplatin through DNA interactions but involving PDT. By connecting Ru(II) to at least one strain-inducing ligand, these complexes become structurally distorted, enabling them to undergo photoinduced ligand loss from triplet metal-centered (^{3}MC) excited states. Theoretically, upon light activation, the strain-inducing ligand is released, leaving behind a ligand-deficient Ru(II) center or liberated ligand, both of which may exhibit cytotoxicity. Ru(II) bonded to two 2,9-dimethyl (2,9-dmp), attached to imidazo[4,5-*f*][1,10]phenanthroline(IP) ligand and appended to a quaterthiophene (4T), known as a Ru-4T, undergoes ligand loss. Alternatively, Ru(II) bonded to two ancillary 1,10-phenanthroline (phen) ligands and an imidazo-[4,5-f] [1,10]phenanthroline (IP) ligand tethered to 4 thienyls, referred to as Ru-4T unsubstituted phen, lacks methyl substituents. The crowding around the metal center is reduced, allowing the molecule to surpass ligand loss upon illumination. Real-time photo NMR experiments have been used to probe the mechanism of action for these revolutionary new medicines in development, and those results will be shared at the upcoming conference.

Speaker

Thomas Williamson

Distinguished Professor | University of North Carolina Wilmington

CSCAN: Conformational Analysis of Macrocyclic Peptides through NMR Chemical Shifts

4:30 PM – 5:00 PM

PANIC

Macrocyclic peptides are increasingly used to bridge the gap between small molecules and biologics in the pharmaceutical industry. Their biological activity and pharmacological properties are governed by conformation, making a detailed understanding of the conformational landscape essential for rational design. Although nuclear magnetic resonance (NMR) is the primary method for determining structures in solution, it remains challenging to apply, especially to N-methylated peptides, because of the scarcity of informative observables such as NOEs, *J*-couplings, and RDCs. To address this challenge, we present a new method for conformational analysis, which we call CSCAN (**C**hemical **S**hift **C**onformational **AN**alysis), based solely on comparing experimental ^{1}H and ^{13}C NMR chemical shifts with theoretical values computed via an efficient workflow combining extensive conformational searches, deep-learning-based geometry refinement, and DFT calculations. Using two pharmaceutically relevant macrocyclic peptides — Cyclosporin A and Aureobasidin A — as examples, we demonstrate that this approach can reliably identify conformations consistent with either X-ray or NMR-based solution structures obtained from NOEs and J-couplings.

Speaker

Alexei Buevich

Principal Scientist | Merck and Co., Inc.

Spin to Win: Embedding Small Molecule NMR in Medicinal Chemistry for Faster Decisions

5:00 PM – 5:30 PM

PANIC

The discovery and optimization of SARS-CoV-2 main protease inhibitors during the Covid-19 pandemic was extremely challenging. The timeline from first synthesis of nirmatrelvir to emergency use authorization (EAU) as an oral antiviral by the FDA was only 17 months. NMR spectroscopy was an essential tool in this process since it can be used to determine the conformation of a small molecule in solution. NMR has proved useful for identifying structural features that may be important for maintaining or improving potency, as well as identifying elements of the compound that impact adsorption. This presentation will describe the discovery and characterization of both the first and second generation, orally bioavailable, SARS-CoV-2 main protease inhibitors from the view of an NMR spectroscopist.

Speaker

Kathleen Farley

Senior Consultant | Solution NMR Analytics LLC

End of Day 1 - Evening on your own

5:30 PM – 5:30 PM

PANIC

Wednesday, May 06, 2026

Breakfast (provided by PANIC)

7:45 AM – 8:45 AM

PANIC

Student Travel Grant Awardee Breakfast with PANIC Leadership

7:45 AM – 8:45 AM

PANIC

PANIC Chair Announcements

8:45 AM – 8:55 AM

PANIC

Bet the Pharm with NMR

8:55 AM – 11:00 AM

PANIC

Session Chair: Luke Arbogast, Subrata Mishra

Speakers


Bruno Garrido

Research Officer | National Research Council Canada


Emily Grasso

Scientist, BioNMR/Protein Bioengineering | NJ Bio, Inc


Daron Freedberg

Senior Scientist | CBER/FDA


Mikhail Reibarkh

Senior Principal Scientist | Merck & Co., Inc.

No-D quantitative NMR of rare natural products using novel solvent suppression methods

9:00 AM – 9:30 AM

PANIC

The non-destructive nature of NMR is invaluable when dealing with rare compounds, allowing samples to be measured and subsequently used, including in the preparation of reference materials. While deuterated solvents are normally used for NMR, this may not always be possible. Compounds such as Caribbean ciguatoxin 5 (C-CTX5) and saxitoxins undergo H/D exchange when dissolved in deuterium enriched solvents and back-exchange can be difficult. Similarly, it was observed that during long-term storage, the aromatic proton in caffeine also undergoes H/D exchange, showing that this issue may be more prevalent than it appears.

No-Deuterium Proton NMR (No-D NMR) [1] provides an alternative to the use of deuterium enriched solvents. We recently introduced solvent suppression approaches that enable No-D qNMR to be performed with high-accuracy [2]. Here we present their application with small amounts of saxitoxin and anatoxin analogues, achieving results that are accurate and traceable in the absence of deuterium enriched solvents. This enables reliable results to be obtained for the production of critically needed reference materials of sample-limited natural products.

References:

1-Hoye et al., Organic Letters 2004 6 (6), 953-956

2-Garrido et al., Analytical Chemistry 2025 97(39), 21240-21248.

Speaker


Bruno Garrido

Research Officer | National Research Council Canada

Assessment of ADC higher-order structure with biomolecular NMR

9:30 AM – 10:00 AM

PANIC

Within the past twenty years, there has been a growing appreciation of the utility of biomolecular NMR in the assessment of biologics at natural abundance. Antibody-drug conjugates (ADCs) are an important class of therapeutics that combine the specificity and stability of antibodies with the enhanced potency of small-molecule payloads. As this field matures, there is an increasing need for novel analytical tools to assess ADC sample quality and provide information about the effects of conjugation upon antibody structure.

In this presentation, I will describe our application of biomolecular NMR to ADC samples to help advance the analytical toolset available for assessment of these therapeutics. Using trastuzumab by itself or conjugated to MMAE or DXd, we collected methyl-selective NMR spectra to assess the higher-order structural features of these systems. At low drug-antibody ratio (DAR), there are strong similarities between the spectra of the unconjugated antibody and the ADCs, but high DAR samples show clear, payload-specific changes relative to the antibody alone. While all spectra of high DAR samples showed site-specific peak broadening, the highest DAR trastuzumab-MMAE spectra also showed global peak broadening and time-dependent changes consistent with aggregation over time, supported by traditional QC metrics. These data highlight the utility of NMR as a tool to assess antibody structural features and its potential to facilitate the development of ADCs.

Speaker


Emily Grasso

Scientist, BioNMR/Protein Bioengineering | NJ Bio, Inc

Improving analytical characterization of conjugate vaccines

10:00 AM – 10:30 AM

PANIC

Conjugate vaccines are highly heterogeneous in terms of glycosylation sites and linked oligosaccharide length. Therefore, the characterization of conjugate vaccines' glycosylation state is challenging. However, improved product characterization can lead to enhancements in product control and product quality. Here, we present a synergistic analytical combination of high-resolution MS (mass spectrometry) and NMR (nuclear magnetic resonance) spectroscopy to analyze glycoconjugates. We demonstrate the power of this strategy using model polysaccharide conjugates to demonstrate a more detailed level of glycoproteomic analysis. This strategy can be readily applied to enhance the characterization of polysaccharide conjugate vaccines. Complete NMR peak assignment and detailed MS information of oxidized oligosialic acid and conjugates are reported. We also show a simple strategy to highlight the oligosaccharide antigen while attenuating peaks from the carrier protein in a glycoprotein. These studies provide a deeper understanding of the conjugation chemistry process and products, which can lead to a better controlled production process.

Speaker

Daron Freedberg

Senior Scientist | CBER/FDA

Novel NMR Approaches for Peptide Conformational Analysis: A Case of cis-Proline Conformation of IPCs Aureobasidin A

10:30 AM – 11:00 AM

PANIC

Aureobasidin A (abA) is a natural depsipeptide that inhibits inositol phosphorylceramide (IPC) synthases with significant broad-spectrum antifungal activity. abA is known to have two distinct conformations in solution corresponding to *trans*- and *cis*-proline (Pro) amide bond rotamers. While the *trans*-Pro conformation has been studied extensively, *cis*-Pro conformers have remained elusive. Conformational properties of cyclic peptides are known to strongly affect both potency and cell permeability, making a comprehensive characterization of abA conformation highly desirable. Here, we report a high-resolution 3D structure of the *cis*-Pro conformer of aureobasidin A elucidated for the first time using a recently developed NMR-driven computational approach. This approach utilizes ForceGen's advanced conformational sampling of cyclic peptides augmented by sparse distance and torsion angle constraints derived from NMR data. The obtained 3D conformational structure of *cis*-Pro abA has been validated using anisotropic residual dipolar coupling measurements. Support for the biological relevance of both the *cis*-Pro and *trans*-Pro abA configurations was obtained through molecular similarity experiments, which showed a significant 3D similarity between NMR-restrained abA conformational ensembles and another IPC synthase inhibitor, pleofungin A. Such ligand-based comparisons can further our understanding of the important steric and electrostatic characteristics of abA and can be utilized in the design of future therapeutics.

Speaker

Mikhail Reibarkh

Senior Principal Scientist | Merck & Co., Inc.

Coffee Break

11:00 AM – 11:25 AM

PANIC

NMR cornucopia

11:25 AM – 1:00 PM

PANIC

The NMR Cornucopia offers a rich assortment of talks that highlight the breadth and versatility of modern magnetic resonance applications. Like a cornucopia, it brings together varying applications into a single session, giving attendees a taste of innovative approaches across the field.

Session Chair: Samuel Kotler

Speakers

Will Pomerantz

Professor of Chemistry | University of Minnesota

Hao Li

Scientist, CMC | Takeda Pharmaceuticals

Robert Evans

Researcher in NMR | University of Manchester

The Promise and Peril of a Maverick Element, Fluorine: Impact on Human Health and the Environment

11:30 AM – 12:00 PM

PANIC

Fluorine-containing molecules have potential for impacting many diverse sectors of industry including their prevalence in human medicine, anesthetics, blood substitutes, agrochemicals, clothing, food packaging, and fire repellents. However, despite the large upside of fluorine, as fluorine forms the strongest of all chemical bonds to the carbon atom, we also encounter highly fluorinated molecules that are persisting in our environment long after their intended use. This persistence has led to their moniker "forever chemicals" or more officially termed poly and perfluorinated alkyl substances (PFAS). This persistence has raised concern about the long-term consequences on human health and the environment.

In this talk, I will discuss some of our approaches studying PFAS, fluorinated pharmaceuticals and agrochemicals, and fluorinated model compounds of functional groups found in bioactive compounds. Using quantitative 19 F NMR and mass spectrometry-based approaches, we quantify total fluorine levels in the environment, and their breakdown under simulated environmental and waste water treatment conditions. These experiments are informing how particular fluorine bonds can be degraded, in some cases forming ultra shortchain fluorinated carboxylic acids (e.g. trifluoroacetic acid), and new safer alternatives designed. Additionally, I will also show how we harnessed a unique property of fluorine to improve our ability to create new imaging tools for 19 F MRI. These results support the importance of the organofluorine bond and its promise for impacting society, while highlighting new areas for innovation when dealing with forever chemicals.

Speaker

Will Pomerantz

Professor of Chemistry | University of Minnesota

Applying NMR to PAT: Structure Elucidation and Mechanistic Insights for Chemical Process Development

12:00 PM – 12:30 PM

PANIC

Process Analytical Technology (PAT) enables improved process understanding, real-time decision-making, and robust control to consistently deliver drug substance quality and manufacturing efficiency. This presentation highlights Takeda's PAT development activities with a focus on Nuclear Magnetic Resonance (NMR) as a versatile platform spanning mechanistic understanding, impurity/degradant characterization, and reaction monitoring across process chemistry development.

High-field NMR (1H/31P/19F)) is showcased for mechanistic and kinetic investigation of reactions, including a challenging amide coupling half-reaction (carboxylic acid activation). Using complementary proton and heteronuclei monitoring, key intermediates are detected and supported by 2D NMR confirmation. Kinetic modeling is used to rationalize pathway competition and explain the observed need for activating agent, informing future optimization strategies (e.g., alternative activating agents and degradation control). In addition, targeted forced degradation case studies demonstrates how NMR-enabled mechanistic understanding and kinetic tracking of process impurities.

Overall, the work illustrates an end-to-end PAT workflow from data acquisition through modeling, and positions NMR as a high-impact technology for Takeda's process chemistry development and manufacturing needs.

Speaker

Hao Li

Scientist, CMC | Takeda Pharmaceuticals

in situ NMR Monitoring of Heterogeneous Reactions

12:30 PM – 1:00 PM

PANIC

NMR spectroscopy can provide valuable insight into chemical reactions, including detailed information on reaction kinetics and mechanisms. While homogeneous reactions are readily studied by *in situ* NMR spectroscopy, studying heterogenous reactions is significantly more challenging since the reaction now takes place at the interface of two, or more, phases. These reactions require well-controlled, efficient mixing to confirm that the observed kinetics are controlled by the reaction rather than by the mass transport between the phases.

Designing and building suitable stirring devices for use within standard NMR spectrometers is a notable challenge. A key restriction is the need to use only NMR-compatible materials, neither magnetic nor electrically conducting, due to the high magnetic fields involved. The tall, narrow shape of standard NMR tubes and the limited available space inside NMR instruments add additional complications, particularly in limiting the effectiveness of mixing. Mixing devices can be either plunger- or stirrer-based.

Our research team has recently developed a stirring device, compatible with most commercial NMR spectrometers. Powered either electrically or pneumatically, a glass shaft is rotated within a standard 5 mm NMR tube, which rapidly stirs the sample. Mixing speeds in excess of 20 kRPM have been achieved. This allows for biphasic reactions, both liquid-liquid and solid-liquid, to be effectively studied, with accurate kinetic data acquired.

Speaker

Robert Evans

Researcher in NMR | University of Manchester

Lunch (provided by PANIC)

1:00 PM – 2:00 PM

PANIC

Posters - Session 2 (odd-numbered) including Coffee Break

2:00 PM – 3:55 PM

PANIC

Poster 1: Leveraging 11B NMR for Optimization of Boronic Acid–Diol Complexation: Insights for SERS-Based Diol Detection (Timmy Nguyen)

Poster 3: A Collaborative Study on Platform 1H Quantitative NMR Method Using Internal Calibration Methodology: Towards Capacity Building for Novices (Sunil Paudel)

Poster 5: Molecular basis of Hsp10-mediated inhibition and disaggregation of α-synuclein amyloid fibrils (Muhammed Shafeek Oliyantakath Hassan)

Poster 7: High Field NMR With a Fully Cryogen-Free, Persistent, Superconducting Magnet (Mathew Brevard)

Poster 9: Tracking the hydration reaction of cementitious calcium silicate hydrate via solid-state NMR (Ray Cowen)

Poster 11: Elucidating the CYP3A4–Midazolam Binding Pose Using Targeted 19F Solid-State NMR and Computational Modeling (Chengming He)

Poster 13: Molecular Characterization of Bilayered Vanadium Oxides for Solid-State Battery Electrodes (Mina Mozafari)

Poster 15: Development of a traceable qNMR certified reference material for external calibration and electronic referencing (Bruno Garrido)

Poster 17: Probing Lipoprotein Particle Size using sPRE with the Functionalized Polyamidoamine (G5-GdBnDOTA) (Mary Starich)

Poster 19: Investigations of E/Z-Conformation for Photoisomerizable 5-Methylene Substituted Hydantoins by EXSIDE NMR and Chemical Shift Analysis (Christopher LeClair)

Poster 21: Expanding the Frontiers of NMR: Advanced Methyl Labeling Strategies for Challenging Therapeutic Targets (Rime Kerfah)

Poster 23: The Development of a Vesicle Model to Study Solvent PRE-Effects on Lipoprotein Particles (Almira Ahmed)

Poster 25: qNMR as a Fingerprinting Tool for Raw Material Characterization (Kaitlyn Doolittle Catlin)

Poster 27: Online benchtop NMR spectroscopy as a PAT tool for monitoring downstream extraction of biosynthesized polyhydroxyalkanoate (Klas Meyer)

Poster 29: Elucidating the Nature of Dynamic Covalent Bonds in Vitrimers with Low- and High-Field NMR (Anya Zornes)

Poster 31: NMR Characterization of Fatty Acid Binding by OBP44a (Mary Starich)

Magic (Angle Spinning): The Gathering

3:55 PM – 5:30 PM

PANIC

Session Chair: Ryan Nieuwendaal

Speakers

Qingzhe Ni

Senior Scientist | Merck

Daria Torodii

postdoctoral researcher | EPFL

Rongfeng Zheng

Senior Scientist | Bristol Myers Squibb

From Milling in small molecule to Lyophilization in vaccine: How solid state NMR Guides Process and Formulation Choices

4:00 PM – 4:30 PM

PANIC

This abstract highlights solid state NMR (ssNMR) as a cross modality analytical technique in pharmaceutical development, spanning small molecule and vaccines. First, we will focus on a small molecule project where ssNMR delivered insight into how milling affects the crystallinity of the sample. It highlighted the phase disorder induced by jet milling and enabled evaluation of stability and annealing. It also provided mechanistic understanding by pinpointing the location of the molecule with the most impact. Combined with thermal analysis (DSC), these results prompted a shift to wet milling for the next GMP campaign. Second, we will focus on a vaccine project in which a lyophilized antigen formulation using a cryoprotectant appears to produce higher molecular weight aggregates, without supporting data to explain why or how this formulation differs. We examined two lyophilized antigen formulations that differed only in their cryoprotectant (cryo1 vs. cyro2) and their respective placebos. By analyzing differences in the cryoprotectant and buffer signals, and sample homogeneity relative to the placebo, the data show decreased amorphous content and increased heterogeneity with cryo1. These results enabled data-driven decisions. As a result, a greater emphasis is placed on cryo2 formulations moving forward. Together, these studies demonstrate ssNMR's breadth in pharma and how enabling data drives process and formulation decisions.

Speaker

Qingzhe Ni

Senior Scientist | Merck

Atomic-Level Structure Determination of Amorphous Drug Formulations

4:30 PM – 5:00 PM

PANIC

The growing interest in amorphous drugs stems from their increased bioavailability, notably allowing more hydrophobic molecules into the drug discovery space. However, such solids are often prone to spontaneous recrystallization during manufacturing, storage or dissolution. The molecular rearrangements leading to recrystallization are difficult to determine *a priori* owing to a lack of atomic level structures. Consequently, a critical step in the development of amorphous drug forms is to determine their stabilization mechanisms at the atomic level.

Recently, the complete three-dimensional atomic-level structures of several amorphous active pharmaceutical ingredients (APIs) have been elucidated by NMR crystallography. Using a combination of NMR, advanced computational methods, and machine learning, we have determined key structural features that lead to the stabilization of these formulations. Here, we outline some of the common structural motifs found in amorphous formulations and relate them to stability. We find that, in contrast to smaller APIs where H-bonding interactions and low-energy conformations that permit such interactions are critical for stability, the main stabilization mechanism in larger molecules (M ~ 1000 g/mol) is the entropic contribution and steric hindrance. To better understand the propensity for crystallization, we compare the structural features observed in amorphous forms to those observed in crystal structures.

Speaker

Daria Torodii

postdoctoral researcher | EPFL

Applications of NMR in Chalcogenide-Stabilized Metal Nanoclusters

5:00 PM – 5:30 PM

PANIC

$Au_{25}(SR)_{18}$ was selected as a model NC to investigate their magnetic properties, with pentanethiol, hexanethiol and octanethiol used as bonding ligands. Both negatively charged and neutral NCs were synthesized, and $^{1}H/^{13}C$ NMR were used for detailed structural analysis, as well as surface bonding ligand environment analyses. The anion NC (diamagnetic) and neutral (paramagnetic) NCs are compared and by using the diamagnetic chemical shifts as references, paramagnetic Knight shifts can be calculated. These shifts measure the spin density along the carbon chain of the surface ligand. Temperature dependent NMR was used to study the spin density effect. Density functional theory calculations were used to predict the spin density on $Au_{25}(SC_8H_{17})_{18}$ and compared with the Knight shifts observed from the experiments. New magnetic properties were observed from the Knight shifts plots. Chalcogenide stabilized NCs, such as with selenolates and tellurolates, have been less investigated, especially their exchange reactions with thiolate. The reaction mechanism, specifically the site preferences and how the mixed ligand layer is distributed on the NCs surface in the exchange reaction, is much less understood. PhSeH and $(PhTe)_2$ were used to exchange $Au_{25}(SC_8H_{17})_{18}$ at different ratios. When the exchange ratio was low, a low exchange extent was observed. With ^{13}C, ^{77}Se, and ^{125}Te NMR, surface ligands’ chemical and electronic environments were studied, as well as the exchange mechanism.

Speaker

Rongfeng Zheng

Senior Scientist | Bristol Myers Squibb

Awards Ceremony

5:30 PM – 6:00 PM

PANIC

BBQ Event

6:00 PM – 8:00 PM

PANIC

Thursday, May 07, 2026

Breakfast (provided by PANIC)

7:45 AM – 8:45 AM

PANIC

Squishy Science from Scalps to Structure

8:45 AM – 10:20 AM

PANIC

Session Chairs: Hattie Ring, Matt Augustine

Speakers

Tyler Meldrum

Associate Professor | William & Mary

Mark Ferris

National Institute of Standards and Technology/CU Boulder

Allison Talley

Senior Scientist | The Procter & Gamble Company

A Mile Wide and Microns Deep: Insights into Materials and Interfaces Through Single-sided Nuclear Magnetic Resonance

8:50 AM – 9:20 AM

PANIC

Single-sided NMR instruments provide an unusual combination of breadth and constraint: they can interrogate real materials *in situ* and nondestructively, yet they access only micron-scale depths. This high-aspect-ratio sensing regime makes them well suited for studying surfaces, polymers, and heterogeneous materials, where interfacial structure and localized dynamics often govern macroscopic behavior. My talk will highlight advances in using single-sided NMR to characterize systems ranging from curing epoxy networks to polymer interfaces, porous media, and other materials with pronounced spatial heterogeneity. I will also explain how relaxation and diffusion measurements obtained using these unconventional instruments can reveal changes in molecular mobility, chemical conversion, and interfacial structure. Emerging directions, including developments aimed at improving sensitivity and contrast, will also be presented. Taken together, these approaches demonstrate that even with microns of penetration depth, single-sided NMR offers a powerful window into the chemistry, physics, and structure of complex materials and their interfaces.

Speaker

Tyler Meldrum

Associate Professor | William & Mary

Single-Sided NMR Profiling of Hydrogel Curing and Conversion

9:20 AM – 9:50 AM

PANIC

Forming soft, biocompatible polymeric materials, e.g. hydrogels, into complex shapes with precise mechanical properties is critical for producing biomedical products such as contact lenses and drug delivery systems, as well as for more advanced products such as artificial organs that might be just a few years away. 3D-printing via vat photopolymerization enables the fabrication of these structures, but light-driven curing produces spatial gradients in polymer conversion that dictates local mechanical and functional properties. Here, the utility of single-sided NMR profiling is demonstrated to fill a metrology gap for techniques that can non-destructively analyze conversion gradients in whole structures printed via vat photopolymerization. A short repetition time, T_1-weighted pulse sequence is used to generate contrast between cured and uncured hydrogel, resulting in an NMR signal contrast that increases linearly with the material's compressive modulus, which is a proxy for conversion. NMR profiling was applied to measure hydrogel cure depth, with the results validated against optical coherence tomography. Finally, full 3D-printed parts were analyzed, revealing differential intra-layer conversion gradients with various layer heights. These results establish single-sided NMR profiling as a versatile, non-destructive tool for analyzing conversion gradients in hydrogels and suggest a pathway toward *in situ* monitoring of vat photopolymerization processes.

Speaker

Mark Ferris

National Institute of Standards and Technology/CU Boulder

Superior Anti-Dandruff Efficacy Predicted with Diffusion NMR Micellar Parameters

9:50 AM – 10:20 AM

PANIC

Dandruff is a pervasive chronic condition which negatively impacts one's quality of life, and effective treatments require efficient delivery of scalp benefit agents. Increased active agent delivery has been shown clinically to result in higher anti-dandruff efficacy as measured by both visible flakes and underlying biomarkers. The delivery of these agents from shampoos requires balancing many technical parameters to achieve the desired outcome without sacrificing secondary parameters, such as cosmetic attributes. We found that two parameters, here termed the Micellar Stability and Micellar Association parameters, predicted increased active agent deposition efficiency and allowed for the design of significantly greater anti-dandruff efficacy. The parameters were quantified via dynamic surface tension and nuclear magnetic resonance (NMR) diffusion measurements on shampoo prototypes and correlated with in vivo scalp measurements. Both surfactant and polymer coacervate-based approaches have been investigated, with decreased micellar stability resulting in more efficient active agent retention on the scalp surface and increased charge density of cationic polymers optimizing coacervation enabling improved active agent delivery. Both approaches can be tuned together or separately for superior performance.

Speaker

Allison Talley

Senior Scientist | The Procter & Gamble Company

Coffee Break

10:20 AM – 10:45 AM

PANIC

High-Octane Resonance: NMR Characterization in the Energy Sector

10:45 AM – 12:20 PM

PANIC

Session Chair: Ryan Nieuwendaal

Speakers

JinHong Chen

Sr. Research Science Consultant | Aramco Americas Company

Asya Arbeli

Postdoctoral Scientist | Columbia University

Qasim Saleem

Research Science Specialist | Saudi Aramco

HSR-NMR Scanning of Slabbed Core

10:50 AM – 11:20 AM

PANIC

The petroleum industry has acquired a massive number of whole cores over the years. The majority of those have been slabbed and plugged/sampled for analysis, then put into storage as slabbed cores. This makes slabbed whole cores the predominant form of cores archived at different core facilities worldwide, and represents a significant asset for advanced analysis to enhance reservoir characterization.

Here we present an optimized high spatial resolution (HSR) measurement method on slabbed cores from unconventional reservoir rocks, using the in-house-developed HSR-NMR scanner. This fit-for-purpose measurement methodology is high-throughput and non-invasive, providing continuous HSR fluid distribution from slabbed cores collected from a well within days. Preliminary results showed that the measured fluid distribution of slabbed source rock cores corelates with the rock structure, organic content, and lamination/bedding, despite challenges presented by missing sections and some subsampling The findings underscore the sensitivity of the HSR-NMR scanner to rock texture, organic content, and bedding. By correlating fluid content and NMR spectra with geological features, HSR-NMR scanning of stored slabbed cores from a well provides continuous basis for quantitative reservoir characterization.

Speaker

JinHong Chen

Sr. Research Science Consultant | Aramco Americas Company

Advancing operando NMR techniques to study degradation processes in commercial Li metal batteries

11:20 AM – 11:50 AM

PANIC

Despite extensive research on Li metal anodes, achieving high Coulombic efficiency remains challenging, and the relationship between surface composition, internal cell pressure, electrolyte chemistry, and electrochemical treatment is still unclear, particularly in practical batteries. Nuclear magnetic resonance (NMR) spectroscopy is a powerful tool for investigating Li metal batteries because it provides quantitative structural, chemical, and dynamical information on solids, liquids, and interfaces with elemental specificity.

However, operando NMR of practical batteries presents challenges due to interactions with metallic casings and internal components, including bulk magnetic susceptibility (BMS), reduced sensitivity, and RF skin depth effects. We show that paramagnetic iron in stainless steel spacers and casings shifts the 7Li NMR resonance to higher frequencies, consistent with simulations, with the effect increasing as more spacers are added. In pouch cells, Ni tabs can further attenuate the signal.

Using newly developed operando NMR hardware compatible with metal-encased batteries, we mitigate signal attenuation and susceptibility artifacts. These measurements enable direct observation of lithium plating and stripping instabilities, monitoring of inactive ("dead") Li formation, and investigation of electrolyte evolution prior to cycling in multilayer pouch and coin cells.

Speaker

Asya Arbeli

Postdoctoral Scientist | Columbia University

Beyond the Borehole: Application of High-Field NMR Spectroscopy in the Oil and Gas Industry

11:50 AM – 12:20 PM

PANIC

NMR spectroscopy in the oil and gas industry is often associated with low-field measurements for well logging and process monitoring. High-field NMR spectroscopy has played a critical, though less apparent, role in enabling molecular-level understanding that underpins technology development and operational troubleshooting across the industrial value chain. This presentation will focus on industrial applications of high-field NMR spectroscopy, demonstrated through a series of case studies spanning upstream, midstream, downstream, and energy-transition activities. Applications of both solution-state and solid-state NMR spectroscopy will be discussed, highlighting how high-field measurements are used to elucidate molecular structure, dynamics, and interactions in mixtures and functional materials relevant to real-world oil and gas operations.

Speaker

Qasim Saleem

Research Science Specialist | Saudi Aramco

Closing of PANIC

12:20 PM – 12:30 PM

PANIC

Lunch PANIC + MANIC

12:30 PM – 1:30 PM

PANIC MANIC

Introductory Remarks

1:30 PM – 1:35 PM

MANIC

Polymers and Soft Materials

1:35 PM – 3:35 PM

MANIC

Speakers

Jeff Reimer

Professor | UC Berkeley

Yu Suzuki

Associate Professor | University of Fukui

Joshua Damron

R&D Staff | Oak Ridge National Laboratory

Tuo Wang

Carl H. Brubaker Professor | Michigan State University

Andrew Korovich

Research Chemist | National Institute of Standards and Technology

Diffusion power spectra as a window into polymer upcycling

1:35 PM – 2:00 PM

MANIC

Spin echoes are now 76 years old, yet they continue to provide a powerful platform for developing new methods to characterize materials. Here we describe how the modulated gradient spin-echo sequence yields frequency-dependent diffusion coefficients that map molecular motion onto polymer dynamics, topology, and chemical state during deconstruction.

When deployed as a multidimensional experiment, this approach reveals exchange of molecular populations across distinct dynamical regimes. We demonstrate these concepts using the swelling-induced acid-catalyzed deconstruction of polydiketoenamine (PDK) polymers. Unexpected features emerge, including the dynamic evolution of configurational entropy and a classical analogue of quantum information science’s paradigmatic test bed for decoherence.

Speaker

Jeff Reimer

Professor | UC Berkeley

Local Structural Roles of Minor Residues in Silk Fibroin Studied by Solid-State NMR: Insights into Fiber Structure Formation

2:00 PM – 2:25 PM

MANIC

Silk fibroin produced by the silkworm *Bombyx mori* consists of a central repetitive sequence region flanked by terminal domains. This repetitive region is composed mainly of GAGAGS or GAGAGA repeats, with some of the A/S residues replaced by Y or V. Silk fibers consist of approximately 60% crystalline regions, separated by less ordered regions generally described as amorphous. The crystalline regions are widely thought to be composed mainly of GAGAGS and GAGAGA repeats, whereas the role of the YV-repeats has not been well understood. Because of the heterogeneous nature of silk fiber, it has been difficult to relate structural features to sequence.

In this study, residue-selective isotope labeling combined with solid-state NMR was used to investigate the conformations of valine and tyrosine residues in both liquid silk prior to spinning and in silk fibers. Quantitative analysis of residue-specific chemical-shift distributions reveals that valine and tyrosine residues adopt secondary structure populations comparable to those of alanine residues. This finding indicates that YV-repeats participate directly in crystalline β-sheet regions rather than being confined to disordered domains. These results imply that YV-repeats form part of the crystalline regions and help define their boundaries, and that the amorphous regions are formed from both AS- and YV-repeats.

Speaker

Yu Suzuki

Associate Professor | University of Fukui

Multiscale NMR Detection of Vitrimer Transitions and Network Dynamics

2:25 PM – 2:50 PM

MANIC

Associative dynamic networks or vitrimers are often assigned a "vitrimer transition" from rheology, but rheological criteria alone are protocol-dependent and can be ambiguous. The extracted transition points vary with frequency window, strain amplitude, heating rate, and sample geometry, while macroscopic flow can conflate bond-exchange dynamics with entanglement and other viscoelastic relaxations. Recently, we have been exploring how solid-state NMR can provide a more direct molecular-level route to identify vitrimer transitions and quantify network dynamics. Low-field 1H NMR tracks temperature-dependent rigid/mobile proton fractions and relaxation behavior, revealing the onset of dynamic heterogeneity and probes effective network constraints as exchange becomes active. High-field 13C solid-state NMR experiments enable site-specific chemical and motional information, linking exchange-active motifs to the mobility changes observed in proton experiments. Together, these measurements decouple segmental softening from topology-conserving bond exchange and provide a robust framework for identifying vitrimer transition behavior beyond rheology. We show the promise of NMR as a probe of vitrimer transitions enabling a more reliable structure-dynamics-processability understanding than rheology alone.

Speaker

Joshua Damron

R&D Staff | Oak Ridge National Laboratory

Solid-State NMR and DNP Reveals Dynamic Lignin-Carbohydrate Architectures Across Plant Development and Carbon Cycling

2:50 PM – 3:15 PM

MANIC

Lignocellulosic biomaterials constitute the largest renewable carbon reservoir on Earth and underpin sustainable materials, bioenergy production, and long-term carbon sequestration. However, resolving their native molecular architecture remains challenging due to structural heterogeneity and limited spectroscopic sensitivity. Here we integrate ^{13}C- and ^{1}H-detected multidimensional solid-state NMR with DNP-enhanced techniques to achieve rapid characterization of intact plant cell walls and complex soil organic matter. These approaches enable in situ mapping of lignin-polysaccharide interactions and precursor-resolved tracking of lignin biosynthesis with substantially improved sensitivity and spectral resolution. Our results reveal that lignin-carbohydrate contacts in plant stems are developmentally staged, with acetylated xylan preferentially associating with syringyl-rich lignin in mature tissues, while methyl-esterified pectin interacts with guaiacyl lignin during early wall formation. Precursor-specific isotope labeling further uncovers distinct routing of phenylalanine and tyrosine into lignin substructures in grasses. Extending these methods to wetland soils formed by degradation of grass residuals identifies pathways of carbon persistence, where preserved aromatic and carbohydrate cores coexist with decomposition-repolymerization products. These studies establish solid-state NMR as a platform for elucidating biopolymers from biosynthesis to long-term carbon fate.

Speaker

Tuo Wang

Carl H. Brubaker Professor | Michigan State University

Characterization of Epoxy Resin Crosslinking for Advanced Semiconductor Packaging via 13C-15N NMR Spectroscopy

3:15 PM – 3:35 PM

MANIC

Modern semiconductor production increasingly utilizes advanced packaging methods, such as multi-chiplet modules and 2.5/3D integrated circuits as a means of increasing transistor counts, performance, and yields, while maintaining or reducing the footprint of the resulting "package". Modern capillary underfill resins often use multiple epoxide and curing agent species to tailor their properties to meet engineering challenges, such as increasingly fine pitch interconnects (<10 μm) and cure-induced stress and shrinkage, complicating efforts to accurately model and predict the cure kinetics and resultant mechanical properties, versus older systems containing simpler formulations. Additionally, the choice of temperature profile can affect the shrinkage and residual stresses in the resulting material, thus understanding the reaction kinetics is of crucial importance.

In this work we aim to develop an open formulation for an epoxy resin test material, alongside new methodologies for characterizing the cure kinetics and mechanical properties critical to packaging optimization and modeling. From ^{1}H solid-echo measurements, we are able to monitor the resin curing *in-situ* via the change in transverse relaxation rate of solid-like cured resin versus uncured material. Through ^{13}C and ^{15}N magic-angle spinning techniques, we can relate these changes to the evolution of specific chemical reactions through the curing process.

Speaker

Andrew Korovich

Research Chemist | National Institute of Standards and Technology

Coffee / Refreshments break

3:35 PM – 4:00 PM

MANIC

Polymers and Soft Materials

4:00 PM – 6:00 PM

MANIC

Speakers

Jacqueline Thomas

Director - Principal Scientist | Procter & Gamble

Toshikazu Miyoshi

Professor | The University of Akron

Linda Reven

Chemistry Professor | McGill University

Eduardo de Azevedo

Prof. | University of São Paulo - Institute of Physics of São Carlos

Ray Cowen

PhD Student | EPFL

Polymer characterization: Measures linked to product performance and current challenges for innovation in industry

4:00 PM – 4:25 PM

MANIC

There are various phases for characterization of polymers, from Discovery and Synthesis, to Use and Performance, to End of Life. Each phase may need different levels of characterization. Various analytical measurement techniques are available to support the different phases from bulk measures to high end measures that pushing the limits of detection. Highlighted will be real examples from P&G focused on Use and Performance showcasing the Analytical Tools used detection, visualization, and recycled packaging. Additionally, current challenges in characterization, such as polymers are often not pure single molecules, but made up of a mixture of like molecules will also be discussed. Approaches will be discussed.

Speaker

Jacqueline Thomas

Director - Principal Scientist | Procter & Gamble

The Importance of Non-crystalline Structure in Polymer Crystallization as Explored by Solid-State NMR

4:25 PM – 4:50 PM

MANIC

2/3 polymers are semicrystalline. Flexibility, connectivity, and topological constraints are intrinsic in polymers and govern crystallization of semicrystalline polymers. In a classical secondary and nucleation theory, polymer chains diffuse into and crystallization proceeds on the existing growth front, where non-crystalline structure was not took into consideration. Characterization of non-crystalline structures is challenging due to the absence of a long-range order. Therefore, the impact of the non-crystalline structure and dynamics has not been considered in polymer crystallization. I will present our recent efforts on characterization of non-crystalline structures of semicrystalline polymers by using solid-state NMR spectroscopy. Poly(Latic acid) (PLA) racemate was used as a model sample. We conducted ^{13}C selective isotope labeling on CH$_3$ of poly(L-Lactic Acid) and CH of Poly(D-Lactic Acid). By using CHHC sequence, we investigated ^{1}H-^{1}H distances between PLA racemates. We could observe structural analogies between non-crystalline and semicrystalline states. This research highlights the importance of an initial non-crystalline precursor into polymer crystallization.

Speaker

Toshikazu Miyoshi

Professor | The University of Akron

Mixed Brush Nanospheres and Nanorods: Self-Assembly via Nanophase separation

4:50 PM – 5:15 PM

MANIC

The spontaneous self-arrangement of immiscible ligands on the surface of nanoparticles (NPs) has been explored as an effective method to form patchy particles, as their self-assembly is of interest for applications in electronics, photonic crystals and catalysis. Synthesis of patchy NPs has been hindered by the difficulty to control the ligand composition and a lack of tools to quantitatively characterize the surface phase separation. Here our previous ligand exchange work for the fabrication of patchy NPs with ZrO$_2$ spherical NPs is extended to stimuli-responsive polymers and NPs of different shapes and compositions. Poly(2-vinyl pyridine) (P2VP) was combined with polyethylene oxide (PEO) and polystyrene (PS) to produce NPs that self-assemble in response to pH and quaternization, similar to their block copolymer counterparts. This method was also applied to non-spherical NPs, TiO$_2$ nanorods. Solution and solid-state NMR experiments demonstrated a wide range of polymer compositions and surface phase separation, while microscopy techniques characterized the assembly structures formed upon selective solvent exposure, pH variation and quaternization. This highly versatile method expands patchy NPs beyond theoretical studies to practical applications as it can be applied to different inorganic cores and polymer combinations to produce well characterized patchy nanoparticles in sufficient quantities.

Speaker

Linda Reven

Chemistry Professor | McGill University

1H Low-Field TD-NMR: From Solid-State and Soft Matter to Porous Media

5:15 PM – 5:40 PM

MANIC

Low-field Time-Domain Nuclear Magnetic Resonance (TD-NMR) has become an important experimental approach for a wide variety of applications. While its early use was largely restricted to relaxation measurements, continuous developments in instrumentation and methodology have substantially extended its capabilities. As a result, TD-NMR is now widely employed for the characterization of material properties, particularly in systems with complex microstructures. In H TD-NMR studies of solid and soft materials, through-space magnetic dipolar couplings between H nuclear spins play a crucial role, rendering the NMR signals highly sensitive to molecular packing and molecular mobility. This intrinsic sensitivity makes H TD-NMR especially effective for identifying mobility transitions, including segmental motions in soft materials, freezing and melting phase transitions, and the dissolution of solids. In this presentation, we will show applications of low-field H TD-NMR in a variety of systems, which includes the study of the molecular dynamics in plastic crystals and polymer composites, as well as to the investigation of the micro- and meso-pore structure of porous materials.

Speaker

Eduardo de Azevedo

Prof. | University of São Paulo - Institute of Physics of São Carlos

Surface-only NMR of calcium silicate hydrate: Advancing surface-selective methods to the atomic-level surface structure of cements

5:40 PM – 6:00 PM

MANIC

Demand for cement, currently over 4 billion tons annually, is projected to continue to grow in the coming decades, driving the need for new, sustainable cements. The development of such cements requires a complete understanding of the structure of the main binding phase, calcium silicate hydrate (CSH). Nuclear magnetic resonance (NMR) spectroscopy has proven to be a powerful tool in the atomic-level study of CSH; from its first use in the 1980s,[1] to the observation of the later stages of the hydration reaction[2] or the determination of the bulk structure of CSH.[3] However, direct experimental probes of the surface structure remain elusive. The extremely thin nature of CSH (~5 nm), and the ubiquity of hydrogen atoms throughout the structure, makes the application of even traditional surface-selective NMR techniques impossible. Here, for the first time, we experimentally differentiate the surface structure from the bulk using new surface-only NMR methods. Through the combination of dynamic nuclear polarization (DNP) methods with selective deuteration, we isolate NMR signals from silicate units originating exclusively at the surface of CSH, thus allowing for characterization of the surface structure. This breakthrough allows for analysis of the surface of CSH and its variants to uncover connections between atomic structure and macro-scale properties.

[1] *Cem. Concr. Res.* **1982**, *12,* 333-339.
[2] *Cem. Concr. Res.* **2004**, *34,* 857-868.
[3] *J. Phys. Chem. C* **2017**, *121* (32), 17188-17196.

Speaker

Ray Cowen

PhD Student | EPFL

Reception & Poster Session

6:00 PM – 8:00 PM

MANIC

Poster 1: Molecular Origins for Thermoplastic Elasticity of Highly Branched Polyethylene as Revealed by Solid-state NMR Spectroscopy (Bohao Peng)

Poster 2: Memory Effect of Crystalline-Chain Dynamics in Semicrystalline Polymer as Revealed by Solid-State NMR (Yuehe Yang)

Poster 3: 19F NMR in the identification and quantification of fluorotelomer alcohols in food packaging materials (Jennifer Janovick)

Poster 4: NMR Analysis of Polymer Homogeneity in Free Radical Polymerization (Meng Wu)

Poster 5: Elucidating the Nature of Dynamic Covalent Bonds in Vitrimers with Low- and High-Field NMR (Anya Zornes)

Poster 6: Leveraging 11B NMR for Optimization of Boronic Acid–Diol Complexation: Insights for SERS-Based Diol Detection (Timmy Nguyen)

Poster 7: Quality Control Assays of Polyurethane Raw Materials Using Benchtop NMR Spectroscopy (Matt Leclerc)

Poster 8: Tracking the hydration reaction of cementitious calcium silicate hydrate via solid-state NMR (Ray Cowen)

Poster 9: Probing molecular exchange in functional materials using variable-temperature 1D NMR and line shape analysis (Shravan Uppala)

Poster 10: Characterizing non-equilibrium self-assembly dynamics of supramolecular polymers using cryo-synchronized reactions (Tianyue Dai)

Poster 11: qNMR as a Fingerprinting Tool for Raw Material Characterization (Kaitlyn Doolittle Catlin)

Poster 12: Transport and Morphology in Molecular Ionic Composite Electrolytes via NMR Diffusometry and Relaxometry (Nicholas Pietra)

Friday, May 08, 2026

Breakfast (provided by MANIC)

7:30 AM – 8:30 AM

MANIC

Energy-Related Materials

8:30 AM – 10:15 AM

MANIC

Speakers

Lauren Marbella

Associate Professor | Columbia University

Jeff White

Professor and BP Chair of Chemical Engineering | Oklahoma State University

Thomas Kress

Research associate | University of Cambridge

Deyang Yu

Senior Research Associate | Virginia Tech

Challenges and Opportunities for Operando NMR of Practical Battery Cells

8:35 AM – 9:00 AM

MANIC

In this talk, discuss our work using operando ^{7}Li NMR to characterize Li deposition morphologies and quantify Li loss modes in multilayer, prismatically-rolled Li metal batteries. While these cells more closely match the active material to electrolyte ratio encountered in practical batteries, the plastic cell casings traditionally used in operando NMR experiments do not mimic the mechanical or thermal properties of real cells. Efforts to acquire NMR on cells used routinely for high throughput and large-scale electrochemical testing encounter significant challenges (e.g., skin depth effects, susceptibility broadening) when used in operando NMR settings. We characterize how practical battery materials (e.g., stainless steel, thick metal casings) impact the observed NMR signal intensities and shifts as well as NMR quantification under operating conditions. From these data, we optimize electrochemical NMR experiments to explore the physical processes that we can probe with this technique, such as metal electrodeposition/dissolution and electrode wetting.

Speaker

Lauren Marbella

Associate Professor | Columbia University

Site Accessibility and Hydrocarbon Reactivity in Zeolites: New Insights from NMR Experiments on a Classic Industrial Catalyst Prepared with Maximum Acidity

9:00 AM – 9:25 AM

MANIC

The faujasite class of zeolites, specifically zeolite Y, are the most widely used catalysts for industrial hydrocarbon processing. In pure and rare-earth exchanged forms, zeolite Y variants are the principal active components in formulated fluid catalytic cracking (FCC) catalysts. While a majority of active sites exist in sterically inaccessible small cages, the locus of catalytic activity has long been considered to be Brønsted acid sites (BAS) located inside the large "supercage" pores of the catalyst. As such, about 60% of potential active sites in these small sodalite cages are ignored based on the fact that even the smallest molecules cannot traverse their ca. 0.26 nm cage openings. Relatively simple and industrially-accessible NMR experiments have shown unexpected findings with respect to this important catalyst. First, catalysts can be prepared with BASs in both the supercage and sodalite cages that very nearly equal the maximum theoretically possible based on framework Al content, in contrast to literature reports, while still preserving structural integrity and eliminating the possibility of associated Lewis acidity. Unexpectedly, hydrocarbon reactivity in both high-temperature cracking reactions and room-temperature isotopic exchange reactions involving bulky hydrocarbons tracks the BAS density *in the inaccessible sodalite cages*, not the accessible supercage sites. NMR methods, reaction kinetics, and implications for catalyst improvements will be discussed.

Speaker

Jeff White

Professor and BP Chair of Chemical Engineering | Oklahoma State University

Probing Ion Transport and Pore Network Connectivity in Nanoporous Carbons Using PFG NMR

9:25 AM – 9:50 AM

MANIC

Ionic transport in nanoporous carbon electrodes strongly influences supercapacitor charge–discharge rates, yet connecting performance to disordered pore architecture is challenging. Using pulsed field gradient (PFG) NMR, we directly measure anion diffusion across multiple length scales to quantify pore-network tortuosity, a key structural descriptor of long-range transport. The measurements reveal a strong discrepancy between short-range diffusion and long-range transport through the pore network: long-range diffusivities correlate closely with high-rate performance, while short-range diffusivities do not. These results highlight PFG NMR as a robust tool for probing complex porous materials and suggest that designing low-tortuosity, well-connected networks is essential for optimizing both transport and electrochemical performance.

Speaker

Thomas Kress

Research associate | University of Cambridge

Comprehensively Probing Ion Transport in Organic-Inorganic Hybrid Electrolytes with Multi-Modal NMR

9:50 AM – 10:15 AM

MANIC

Lithium batteries are complex, multiphase systems in which the kinetics of Li^+ transport govern the rates of energy storage and release. Quantifying the various Li^+ transport modes in such heterogeneous environments, however, remains challenging. Here, we demonstrate how advanced NMR techniques can elucidate ion transport in organic-inorganic hybrid electrolytes, prepared by dispersing Li^+-conducting inorganic particles into surrounding electrolytes composed of lithium salts and organic solvents or polymers. Using a combination of NMR diffusometry, electrophoretic NMR, and dynamic NMR, together with impedance spectroscopy, we systematically resolve different ion transport modes in these hybrid electrolytes. This integrated approach allows us to quantify 1) the contribution of each phase to the overall ionic conductivity, 2) the interfacial resistance associated with Li^+ transport through the organic/inorganic interfaces, 3) the Li^+ transference number of the hybrid electrolytes, and 4) most importantly, the kinetics of Li^+ exchange at the interfaces. These NMR-enabled insights provide a mechanistic framework for understanding ion transport in hybrid electrolytes and offer new design principles for polymer-ceramic composite electrolytes in solid-state batteries.

Speaker

Deyang Yu

Senior Research Associate | Virginia Tech

Coffee / Refreshments break

10:15 AM – 10:45 AM

MANIC

Energy-Related Materials

10:45 AM – 12:00 PM

MANIC

Speakers

Michael Ryan Hansen

Professor | Insitute for Physical Chemistry, University of Münster, Germany

Ying Chen

Materials Scientist | Pacific Northwest National Laboratory

Alexej Jerschow

Professor | New York University

Multinuclear Solid-State NMR: A Spectroscopic Window into the Molecular World of Battery Materials

10:45 AM – 11:10 AM

MANIC

Understanding the function of battery materials at the molecular level is an important step towards the development of the next-generation, high-performance batteries. Solid-state NMR spectroscopy represents a key method for revealing such molecular details, capable of analyzing both disordered and ordered materials even under operando conditions. Inorganic solid electrolytes have emerged as an alternative to liquid electrolytes, offering improved ion migration through modifications to the metallic cations within the solid electrolyte framework. Likewise, lithium alloying materials are considered promising candidates as negative electrode materials in lithium-ion batteries due to their high specific capacity and relatively low cost. However, revealing how such materials become lithiated based on their state of charge is challenging. In this contribution, I will provide examples from our recent research on ion migration in superionic Li- and Na-based inorganic solid electrolytes and thermoelectric materials. Furthermore, we have conducted studies on the lithiation mechanism for various Sn-electrode materials.

Speaker

Michael Ryan Hansen

Professor | Insitute for Physical Chemistry, University of Münster, Germany

Magnetic Resonance Insights into Organic Cathode Materials and Non-Classical Nucleation Pathways

11:10 AM – 11:35 AM

MANIC

Redox-active organic materials hold great potential as electrode materials for next-generation batteries due to their low cost, high theoretical capacity, and synthetic tunability. By combing solid- and solution-state NMR with CW and pulse EPR methods, we obtained detailed structural and radical speciation information for two tetraaminobenzoquinone cathode materials, revealing that a well-ordered hydrogen-bonding network is correlated with a multi-order-of-magnitude increase in electroconductivity.

Beyond energy storage materials, NMR also provides unique opportunities to uncover transient pre-nucleation species. Using operando solution- and solid-state NMR, we observed the transformation of Ca·HCO$_3$ ion pairs into a Ca·HCO$_3$ dense liquid phase (DLP), followed by the decomposition reaction of the DLP to hydrated ACC. Additionally, combined in situ and ex situ solid-state ^{27}Al multiple quantum magic angle spinning (MQMAS) NMR demonstrates that a large, purely hexa-coordinated aluminum cluster forms directly from amorphous aluminum hydroxide gel and converts to gibbsite via the release of Al-O monomers, whereas tetra-coordinated clusters serve as intermediates that do not transform into the crystalline phase. Together, these examples highlight the power of NMR and EPR to resolve local structure, radical chemistry, and transient intermediates, providing molecular-level insight into both functional energy materials and non-classical nucleation pathways.

Speaker

Ying Chen

Materials Scientist | Pacific Northwest National Laboratory

From Rechargeable Battery Diagnostics to Molecular Dynamics

11:35 AM – 12:00 PM

MANIC

Rechargeable batteries pose significant challenges for nondestructive characterization due to their complex internal dynamics and failure mechanisms. We present advanced diagnostic approaches that leverage magnetic resonance and magnetometry techniques, complemented by molecular dynamics (MD) simulations, to provide deep insights into battery processes across multiple length and time scales. MRI-based methods enable fast, spatially resolved, nondestructive scanning of full cells, allowing sensitive determination of site-resolved state-of-charge, current distributions, early defect detection, and electrode chemistry changes during charge/discharge cycles. To further elucidate underlying dynamic processes, we integrate NMR spectroscopy, which probes motions over wide timescales (ps to µs) via relaxation rates, with MD simulations. This synergy enables rigorous untangling of relaxation mechanisms, elucidating dynamical models on molecular scales, and enhancing signal assignment. Recent extensions include tracking sodium ions in hydrogel-based desalination materials. Overall, the combined use of MRI, magnetometry, advanced NMR, and MD simulations provide powerful methodologies for fundamental electrochemical research, and accelerated development of next-generation of materials and devices.

Speaker

Alexej Jerschow

Professor | New York University

Lunch and Poster session

12:00 PM – 1:30 PM

MANIC

Poster 1: Molecular Origins for Thermoplastic Elasticity of Highly Branched Polyethylene as Revealed by Solid-state NMR

Spectroscopy (Bohao Peng)

Poster 2: Memory Effect of Crystalline-Chain Dynamics in Semicrystalline Polymer as Revealed by Solid-State NMR (Yuehe Yang)

Poster 3: 19F NMR in the identification and quantification of fluorotelomer alcohols in food packaging materials (Jennifer Janovick)

Poster 4: NMR Analysis of Polymer Homogeneity in Free Radical Polymerization (Meng Wu)

Poster 5: Elucidating the Nature of Dynamic Covalent Bonds in Vitrimers with Low- and High-Field NMR (Anya Zornes)

Poster 6: Leveraging 11B NMR for Optimization of Boronic Acid–Diol Complexation: Insights for SERS-Based Diol Detection (Timmy Nguyen)

Poster 7: Quality Control Assays of Polyurethane Raw Materials Using Benchtop NMR Spectroscopy (Matt Leclerc)

Poster 8: Tracking the hydration reaction of cementitious calcium silicate hydrate via solid-state NMR (Ray Cowen)

Poster 9: Probing molecular exchange in functional materials using variable-temperature 1D NMR and line shape analysis (Shravan Uppala)

Poster 10: Characterizing non-equilibrium self-assembly dynamics of supramolecular polymers using cryo-synchronized reactions (Tianyue Dai)

Poster 11: qNMR as a Fingerprinting Tool for Raw Material Characterization (Kaitlyn Doolittle Catlin)

Poster 12: Transport and Morphology in Molecular Ionic Composite Electrolytes via NMR Diffusometry and Relaxometry (Nicholas Pietra)

Materials Methods and Polymers

1:30 PM – 3:25 PM

MANIC

Speakers

Leah Casabianca

Professor | Clemson University

Atsushi Asano

Professor | Department of Applied Chemistry, National Defense Academy

Aaron Rossini

Professor | Iowa State University

Timmy Nguyen

Graduate Student | University of Minnesota

Rebecca Martin

Graduate student | Virginia Tech

NMR Techniques for Understanding Interactions Between Nanoscale Plastic Particles and Other Environmental Pollutants

1:30 PM – 1:55 PM

MANIC

Micro- and nanoscale plastic (MNP) results from the breakdown of larger plastic pieces in the environment. Due to their large and highly reactive surface area, MNP particles can absorb and sequester toxic small molecules that may also be present in polluted waterways. One class of these small molecules are per- and polyfluorinated alkyl substances (PFAS). These compounds contain CF_2 and CF_3 groups, and are persistent in the environment due to the strength of the C-F bond. There are not many techniques available that can probe the detailed structure and dynamics of the interactions between PFAS and MNP in an aqueous environment. However, NMR is uniquely poised to be able to answer these important questions. Here we will present recent work using a set of complementary solution-state NMR techniques to identify and characterize binding between PFAS and MNP.

Speaker

Leah Casabianca

Professor | Clemson University

Nanophase Structure of Polyurea-based Materials investigated by Solid State NMR

1:55 PM – 2:20 PM

MANIC

I present two topics; one is analysis of nanoscale phase separation in a self-healable poly(octamethylene thiourea) ($PTUC_8$)/poly(ether thiourea) ($PTUEG_3$) blend, and the other is the identification of the broken regions in polymer chains during tharmal degradation of poly(urea urethane) (PUU).

$PTUEG_3$ exhibits excellent mechanical robustness and shows self-healing ability even at temperatures below its glass transition temperature. In contrast, $PTUC_8$, a one-dimensional structural analogue of $PTUEG_3$, does not exhibit self-healing ability. Blends with $PTUC_8$/$PTUEG_3$ ratios from 50/50 to 80/20 exhibited self-healing behavior, whereas the 90/10 blend did not. The ^1H T_{1r} analyses revealed nanophase separation on a few nm in the 50/50 to 80/20 blends.[1] These results suggest that nanophase separation is a key factor in exhibiting self-healing ability.

Chain scission and crosslinking in PUU, widely used in heat-insulating materials and shoe soles, occur at urea and urethane linkages during aging, leading to changes in tensile strength and elongation behavior. To evaluate service lifetime, the ^{13}C and ^{15}N NMR analyses were conducted during thermal aging to characterize degradation behavior, complemented by ^1H T_2 analysis.[2]

1. Fujisawa, Y., Nan, Y., Asano, A., Yanagisawa, Y., Kano, K., Itoh, Y., Aida, T. *Angew. Chem. Int. Ed.*, 2023, **62**(5), e202214444.

2. Numata, K., Asano, A., Nakazawa, Y. *Polm. Deg. Stab.*, 2020, **172**, 109052.

Speaker

Atsushi Asano

Professor | Department of Applied Chemistry, National Defense Academy

Structure Determination of Semiconductor Nanocrystals by Dynamic Nuclear Polarization (DNP) Solid-State Nuclear Magnetic Resonance

2:20 PM – 2:45 PM

MANIC

Semiconductor nanocrystals (NCs) have uses in lighting and displays, photovoltaics, catalysis and bio-sensing. Due to their small particle diameters, typically 10 nm or less, the fraction of atoms residing on the surface of the NC is sizeable. The surface structure strongly influences the photophysical properties of these materials. Therefore, there is a need for analytical techniques that can probe the structure of surface atoms. In this talk I will describe how high-resolution solid-state NMR spectroscopy with sensitivity enhancement by dynamic nuclear polarization (DNP) can be used for the precise structure characterization of CdSe NCs. CdSe NCs are a prototypical material and also feature two spin-1/2 isotopes (^{113}Cd and ^{77}Se) which are amenable to NMR spectroscopy. I will show how with DNP it is possible to enhance the sensitivity of solid-state NMR experiments on CdSe nanocrystals by one to two orders of magnitude. These sensitivity gains enable a variety of otherwise impossible NMR experiments. Examples of NMR experiments that will be described include ^{13}C, ^{15}N, ^{35}Cl, ^{77}Se and ^{113}Cd homonuclear and heteronuclear 2D correlation NMR experiments. With these NMR experiments detailed atomistic models of NCs can be obtained.

Speaker

Aaron Rossini

Professor | Iowa State University

Leveraging 11B NMR for Optimization of Boronic Acid–Diol Complexation: Insights for SERS-Based Diol Detection

2:45 PM – 3:05 PM

MANIC

Boronic acids (BAs) are well-known for their ability to form reversible, covalent bonds with 1,2- and 1,3-diols, making them valuable capture agents to facilitate detection of biologically relevant diols. While their integration with surface-enhanced Raman spectroscopy (SERS) holds promise for selective analyte localization, their applications beyond saccharide detection remain limited. This is largely due to the time-consuming optimization required to establish ideal diol-binding conditions. Herein, this work explores the use of 11B NMR spectroscopy with SERS to efficiently optimize small-molecule BA capture agents for diol detection. 11B NMR offers an efficient method for rapidly assessing the BA pKa and binding affinity, which can be applied to enhance the performance of the SERS-based sensor. The diol reactivity of 4-mercaptophenylboronic acid and 2-aminopyrimidine-5-boronic acid was assessed with cyclopentanediol and catechol as model diols across a range of pH conditions and concentrations. The 11B NMR spectra provide both qualitative insight into the structure of the product complex and quantitative determination of binding affinity. Subsequent SERS measurements confirm that the highest binding affinity occurs at the pH predicted by 11B NMR. By coupling simple molecular-based characterization with complementary surface-based detection, this approach streamlines the development of BA-based biosensors to expand their applicability for other biologically relevant diols.

Speaker

Timmy Nguyen

Graduate Student | University of Minnesota

Natural abundance 13C quantification of CO2 transport and sorption in molecular ionic composite gas separation materials

3:05 PM – 3:25 PM

MANIC

Gas separations represent critical processes in applications including air purification for human space travel, carbon capture, and natural gas purification. We have created molecular ionic composite (MIC) materials for stable, regenerable, and selective gas sorption. MICs are a class of materials formed from a rigid, double-helical, sulfonated-polyaramid polymer combined with ionic liquids (IL) or other polar or ionic species. MICs promise to provide an energy-efficient, high capacity, and robust alternative to, for example, pumped-liquid-based CO_2 scrubbers for power plant flue gas. We developed a convenient method for NMR analysis by natural abundance CO_2 sorption into MICs using dry ice. Incorporating optimized concentrations of T_1 relaxation agents enables precise quantification of CO_2 gas sorption and transport in minutes to hours using high resolution ^{13}C NMR spectroscopy and diffusometry. ^{13}C NMR quantifies CO_2 loadings of 1-5 wt% in liquid (IL) and solid (MIC) samples and diffusion rates that are ~10X faster than the component ions in MICs (measured by ^{1}H and ^{19}F NMR). These solid-composite sorption materials can be widely and predictively tuned to positively impact target gas solubility and selectivity. The use of NMR in analysis of gas separation/sorption materials represents an information-rich and versatile platform to gain insights into selective transport properties and correlations with material structure and dynamics.

Speaker

Rebecca Martin

Graduate student | Virginia Tech

Coffee / Refreshments break

3:25 PM – 3:55 PM

MANIC

Materials Methods and Polymers

3:55 PM – 5:50 PM

MANIC

Speakers

Klaus Schmidt-Rohr

Professor of Chemistry | Brandeis University

Mark McCormick

NMR Spectroscopist | 3M

Amrit Venkatesh

Assistant Professor of Chemistry | University of Virginia

Jay Baltisberger

Senior Chemist | Wacker Chemical Corporation

Yuehe Yang

Student | The University of Akron

Elucidating the Structure of COFs, Organic Electrode Materials, and Biodegradable Polyesters by ssNMR

3:55 PM – 4:20 PM

MANIC

Solid-state NMR is the best available method for characterizing the structure of insoluble organic materials. Nevertheless, due to distorted peak intensities, peak splittings from packing effects, and wishful thinking, routine ^{13}C ssNMR spectra of insoluble materials are sometimes misinterpreted. Two examples will be discussed. Based on multiCP ^{13}C & ^{15}N spectra, we show that a promising "COF" is not a framework at all. Secondly, in a tricyclic electrode material used in Li-ion batteries, quantitative direct-polarization (DP) ^{13}C & ^{15}N spectra with ^{1}H dipolar dephasing show that central N atoms are not bonded to H, invalidating the structure presented in several high-profile publications. Fast T_1 relaxation due to unpaired electrons makes DP the best choice for quantitative NMR. Peak splittings are shown to be due to symmetry-breaking H-bonding.

In biodegradable PE-like polyesters made with $^{13}C_2$-ethylene glycol, NMR can characterize the crystalline chain conformation through tensor correlation and the crystallite thickness through ^{1}H spin diffusion. NMR reveals several types of O-induced *gauche* conformations in the crystallites and at the interface. For long diacids, the diesters exclusively form interfacial layers, so N controls the crystallite thickness. Double kinks in crystalline diol segments deduced from 2D NMR have been confirmed by XRD. Dynamic *gauche*$^+$/*gauche*$^-$ disorder and associated increased entropy in the crystallites for N = 18 raises the melting point by ≥10 K.

Speaker

Klaus Schmidt-Rohr

Professor of Chemistry | Brandeis University

Characterization of Tackified Silicone Adhesives

4:20 PM – 4:45 PM

MANIC

Silicone adhesives are a vital part of 3M's product portfolio. Tackifiers are commonly used to modify the rheological properties of adhesives to tune their use for different applications. We use solid-state NMR at high and low field to probe the structure and dynamics of tackified silicone adhesives. Questions on network properties, phase separation, and dynamics are probed.

Speaker

Mark McCormick

NMR Spectroscopist | 3M

High-Resolution Fluorine-19 Solid-State NMR Spectroscopy for Materials Characterization

4:45 PM – 5:10 PM

MANIC

Solid-state nuclear magnetic resonance (NMR) spectroscopy can probe complex heterogeneous materials with high fidelity, where other techniques offer limited information. In materials containing fluorine, ^{19}F solid-state NMR spectroscopy is a sensitive probe of its local chemical environment due to its high Larmor frequency, high natural abundance, and broad chemical shift range of ca. 700 ppm. Consequently, ^{19}F NMR offers the ability to investigate minute changes in local structure, measure intermolecular interactions, and probe molecular confinement. However, the resolution of ^{19}F solid-state NMR can be severely limited due to large chemical shift anisotropy, homonuclear ^{19}F-^{19}F and heteronuclear ^{1}H-^{19}F dipolar couplings.

Here, we present two approaches to mitigate this problem and obtain high-resolution ^{19}F solid-state NMR spectra with examples of applications in catalysis and pharmaceuticals. We apply fast magic angle spinning to improve ^{19}F spectral resolution, allowing us to probe self-assembled nanomaterials, confinement in zeolites and polymer-based heterogeneous catalysis supports. Alternatively, in highly protonated systems like organic pharmaceuticals, ^{1}H decoupling offers significant enhancement in resolution. We leverage this resolution enhancement to characterize multi-component solid active pharmaceutical ingredients. These examples demonstrate the utility of high resolution ^{19}F solid-state NMR spectroscopy in heterogeneous catalysis and pharmaceuticals science.

Speaker

Amrit Venkatesh

Assistant Professor of Chemistry | University of Virginia

PIETA for all - pulse sequence and processing improvements

5:10 PM – 5:30 PM

MANIC

The Grandinetti lab introduced[1] the Phase Incremented Echo Train Acquisition (PIETA) approach that could be applied to a variety of experiments where CPMG-like echo trains were acquired and phase coherence fidelity was required. Recently the PIETA method[2] was used to acquire single-shot J-resolved 2D spectra from zeolites to determine crystal structures of the materials, providing motivation for others to try the experiment. In the last few years, the sequence has been improved so that it is possible to remove the phase dimensions from the experiment and process the data easily. Changes made to the sequence and processing will be discussed, including using adiabatic pulses in liquid state to perform PIETA experiments. The implementation returns to a very simple idea that the receiver phase on an NMR spectrometer has two phase components, one for how complex data is coadded and the other for the mixing RF phase. By explicitly setting the RF phase using real-time pulse sequence mathematics for each echo in the train, PIETA can be implemented without requiring processing of phase dimensions. These modified sequences will allow many more researchers to address problems across a wide range of areas using PIETA.

1. Baltisberger, J.H. *et al.* PIETA in NMR spectroscopy. *J. Chem. Phys.* **136**, 211104 (2012)
2. Srivastava, D.J. *et al.* Refining siliceous zeolite framework structures with ^{29}Si 2D *J*-resolved NMR spectroscopy. *Phys. Chem. Chem. Phys.* **27**, 419–435 (2025)

Speaker

Jay Baltisberger

Senior Chemist | Wacker Chemical Corporation

Memory Effect of Crystalline-Chain Dynamics in Semicrystalline Polymer as Revealed by Solid-State NMR

5:30 PM – 5:50 PM

MANIC

α_c mobile polymer crystals conduct crystalline chain dynamics below melting temperature (T_m) in addition to segmental motions in the amorphous region above glass transition temperature (T_g). The crystalline chain dynamics involves translations and rotations of the crystalline segment which result in chain diffusion between the crystalline and amorphous regions. Crystalline chain dynamics play significant roles into re-organizations during crystallization/annealing as well as deformations. However, the impacts of crystalline, amorphous and interfacial structures on crystalline chains dynamics is not well understood. In this study, we investigate detailed crystalline chains dynamics of poly(L-lactic acid) in solution- and melt-grown crystals by using solid-state NMR spectroscopy. Temperature-dependent CODEX build-up curves determined that melt-grown crystals show a lower Ea(95 kJ/mol) than solution-grown crystals Ea(126 kJ/mol). We further investigated correlations of individual jumps by using site-specific two-dimensional exchange NMR. The buildup curves were analyzed in terms of Markovian random-walk, one-directional sliding, locally confined three sites, and their combinations. It was revealed that the dynamics correlations deviate from Markovian movement and has a higher probability to return to the original site (memory effect). We will discuss the impacts of morphology and molecular weight on the memory effect of crystalline chain dynamics.

Speaker

Yuehe Yang

Student | The University of Akron

End of MANIC

5:50 PM – 5:50 PM

MANIC

Dinner (off site)

6:30 PM – 6:30 PM

MANIC