Conference Program (as of April 15, 2023)

This Conference Program is subject to change. It is intended to serve as a reference guide only.

The online planner and mobile app tools will be available in late March.
These tools are for registered attendees and will be updated regularly as changes occur.

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64th ENC PROGRAM (as of April 15, 2023)
This program is subject to change.

SATURDAY, APRIL 15

Pre-Conference Vendor Meetings
Times & Locations Vary

09:00-16:30, **IVAN Meeting**, Oak Shelter bldg on Asilomar campus – **Learn More** & **RSVP Today**

13:00-17:00, **Bruker Workshops**, Monterey Plaza & Spa - **Learn More & RSVP Today**

SUNDAY, APRIL 16

Pre-Conference Vendor Meetings
08:00-14:15

8:30-12:30, **Bruker Symposium**, Monterey Plaza & Spa, **Learn More & RSVP Today**

08:00-13:00, **JEOL NMR Mini-Symposium**, Fred Farr bldg on Asilomar Campus - **Learn More & RSVP Today**

12:30-14:15, **ACD/Labs Meeting**, Nautilus bldg on Asilomar Campus – **Learn More & RSVP Today**

Conference Check-in/ Name Badge Pick Up
10:00-18:00, Triton

YOUNG SCIENTISTS' SYMPOSIUM (YSS)
14:30-16:00, Merrill Hall

YSS 14:30, **Jihyun Kim** (Weizmann Institute of Science) New cross-polarization schemes for heteronuclear transfers involving labile protons in biomolecular NMR		YSS 15:15, **Shannon L Eriksson** (Duke University) Improving SABRE Polarization Through Three-Dimensional Magnetic Field Manipulation
YSS 14:45, **Wenkai Zhu** (University of Pittsburgh) Visualizing Proteins in Mammalian Cells by 19F NMR Spectroscopy		YSS 15:30, **Haiyan Mao** (University of California, Berkeley) Scalable nanoporous networks for carbon capture via solid-state NMR spectroscopy
YSS 15:00, **Nuwandi M. Ariyasingha** (Wayne State University) Efficient Polarization Re-distribution in Hyperpolarized Propane Produced Via Pairwise Parahydrogen Addition		YSS 15:45, **James J. Kimball** (Florida State University) Broadband Adiabatic Inversion Cross-Polarization: Theory and Applications

WELCOME RECEPTION with Exhibit Booths & Young Scientist Posters – **All Attendees Invited**
16:00-18:00, Fireside Pavilion

ASILOMAR LODGER DINNER for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees may purchase a lunch ticket bundle or dinner ticket online by April 7.
18:00 – 19:00, Crocker Dinning Hall

OPTIONAL Vendor Hospitality Suites (following reception)

MONDAY, APRIL 17, 2023

Early Morning Lecture Series (for Students & ALL who wish to learn!)
07:00-07:50, Merrill Hall

07:00-07:50 **Understanding NMR Spectroscopy** Part 1 of 4

Presenter: James Keeler

Would you like to deepen or brush up your understanding of NMR theory? Join us for a morning lecture series by **James Keeler** (University of Cambridge), author of *Understanding NMR Spectroscopy*. These lectures assume only a modest prior knowledge of NMR theory and will cover some key topics of wide interest to budding NMR spectroscopists. Topics will include: Energy levels, Hamiltonians and operators; Introducing and using product operators; Relaxation; Coherence selection by phase cycling and field gradients

ASILOMAR LODGER BREAKFAST for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees cannot purchase breakfast tickets, but you can purchase lunch and dinner tickets by April 7.
07:30-09:00, Crocker Dining Hall

MOA: Laukien Prize Session (plenary session)
08:45 -10:10, Merrill Hall
Len Mueller and Daniel Raftery presiding

COFFEE BREAK with Exhibit Booths and Posters, Fireside Pavilion
10:10-10:45

MOD: Hyperpolarization & Eclectica (parallel session)
10:45-12:35, Merrill Hall

10:45-11:10 **Tracking Degradation in Commercial Li Batteries with High Chemical and Temporal Resolution**

Presenting Author: Lauren Marbella

Lauren Marbella (Columbia University)

Anode-free batteries offer the highest specific energy density for Li-based batteries, but practical application is plagued by the growth of high surface area Li deposits. The presence of these Li filaments is strongly correlated with the formation of dead (electrochemically inactive) Li that leads to low Coulombic efficiency (CE) and serious safety concerns. Yet, electrifying large-scale modes of transportation will rely on energy dense technologies. Commercial batteries present unique challenges because the way that electrodes are stacked inside of a multilayer cell impact Li deposition due to differences in pressure in the system. I will discuss our efforts to use operando NMR spectroscopy to probe buried interfaces in these systems and quantitatively detect Li growth, dead Li, and electrolyte decomposition.

MONDAY, APRIL 17, 2023 - *continued*

11:10-11:30 **Toward Efficient SABRE Hyperpolarization of Tin-117 Nuclear Targets for Neutron Optics-Based Time-Reversal Symmetry Investigations**

Presenting Author: Abubakar Abdurraheem

Abubakar Abdurraheem (Wayne State University); Shahabuddin Alam (Southern Illinois University); Anthony Petrilla (Southern Illinois University); Boyd Goodson (Southern Illinois University); Roman Shchepin (South Dakota School of Mines and Technology); Michale Snow (Indiana University/CEEM); Eduard Chekmenev (Wayne State University)

Tin-117 has been identified as a nucleus of interest for envisioned neutron-optics based searches for time-reversal invariance violation (TRIV). However, such experiments would require the sustained production of large quantities of hyperpolarized 117Sn nuclei on a neutron beam line. We report on our pilot efforts to prepare HP states in another spin-1/2 tin isotope, 119Sn, using SABRE hyperpolarization and detection with a benchtop NMR spectrometer capable of detecting both tin isotopes. The spectrometer detects 119Sn with greater sensitivity, facilitating substrate hyperpolarization screening with the rationale that our observations may be expanded to 117Sn hyperpolarization. 119Sn polarization is relayed through 1H substrate spins, and can be hyperpolarized in tin-functionalized pyrimidine, imidazole, and oxazole rings; oxazole derivatives yielded the highest proton polarization.

11:30-11:50 **First demonstration of SABRE hyperpolarized 1-13C Pyruvate metabolism detected in vivo**

Presenting Author: Austin Browning

Austin Browning (North Carolina State University); Keilian MacCulloch (North Carolina State University); Matt Rosen (MGH/Martinos Center); Eduard Chekmenev (Wayne State University); Boyd Goodson (Southern Illinois University); Thomas Theis (North Carolina State University); Patrick TomHon (Vizma Life Sciences); Carlos Dedesma (Vizma Life Sciences); Yi-Fen Yen (Harvard Medical School); David Bedoya (Harvard Medical School)

The first SABRE hyperpolarized in-vivo signal is shown here with 1-13C Pyruvate as the metabolite. The 1-13C Pyruvate signal last for over a minute, with a 20° flip angle, while the metabolic conversion to 1-13C Lactate is highlighted, with a 30° flip angle. This work was performed using our variable field MRI, set to 1.5 T. The next step in this work is moving to a biocompatible solution to allow for survival based studies utilizing SABRE and CSI to monitor diseased and healthy models for location and conversion rates of pyruvate and lactate. What this current work shows is a clear "giant leap" and path forward for the use of the simple and cost-effective method of SABRE for in-vivo applications.

11:50-12:10 **Co-hyperpolarized [13C,15N2]Urea + [1-13C]Pyruvate for Perfusion and Metabolic Imaging of Human Abdomen**

Presenting Author: Yaewon Kim

Yaewon Kim (University of California); Hsin-Yu Chen (University of California); Tanner Nickles (University of California); Jeremy Gordon (University of California); Peder Larson (University of California); Xiaoxi Liu (University of California); Louise Magat (University of California); Philip Lee (University of California); Daniel Gebrezgiabhier (University of California); Cornelius von Morze (Washington University); Daniel B. Vigneron (University of California); Michael A. Ohliger (University of California)

[13C,15N2]Urea and [1-13C]pyruvate were co-polarized using dynamic nuclear polarization and injected into healthy volunteers for simultaneous imaging of perfusion and metabolism in the abdomen. Whole-abdomen dynamic images were successfully obtained, and the distribution of urea was compared to pyruvate and its metabolites. While relative intensities in various organs were similar between urea and pyruvate, the time-to-peak of urea was earlier than pyruvate in kidneys and spleen. These effects may reflect differences in vascularity, permeability and metabolism for the two agents. This study investigated the first use of co-polarized HP pyruvate and urea in the human abdomen and demonstrated clinical-research value for simultaneous perfusion and metabolic imaging in abdominal organs and future MR molecular imaging of tumors and metabolic diseases.

12:10-12:35 **MRI of Roots in the Greenhouse and Agricultural Field**

Presenting Author: Hilary Fabich

Hilary Fabich (ABQMR, Inc.)

Analyzing plants above the ground is routine in plant breeding programs. Though the roots are an essential part of the plant, there is no convenient method for studying intact roots in natural soil. We have developed low-field MRI systems for use both in the greenhouse and agricultural field. The systems can be transported around the agricultural field and acquire 3D images of intact roots in natural soils. In addition to hardware development, we have been working to optimize pulse sequences to separate the signal of soil water from that of root water. Being able to image the root architecture provides useful information for plant breeders as they breed plants for specific climates and disease resistance.

MONDAY, APRIL 17, 2023 - *continued*

MOE: MRI: Methods and Applications (parallel session)
10:45-12:30, Chapel

10:45-11:10 **K2S Challenge: From Undersampled K-Space to Automatic Segmentation**

Presenting Author: Valentina Pedoia

Valentina Pedoia (UCSF)

Image reconstruction and downstream tasks have typically been treated independently by the image processing community, but we hypothesized performing them end-to-end facilitate further optimization. To these ends, UCSF organized the K2S challenge, where challenge participants were tasked with segmenting bone and cartilage from 8X undersampled knee MRI acquisitions. Top challenge submissions produced high-quality segmentations maintaining fidelity to ground truth, but strong reconstruction performance proved not to be required for accurate tissue segmentation. This, in conjunction with there being no correlation between reconstruction and segmentation performance, confirmed reconstruction algorithms can be optimized for downstream tasks in an end-to-end fashion.

11:10-11:30 ***in vivo* Imaging Stroke via 3D Hyperpolarized Xenon MRI with hundreds micron resolution**

Presenting Author: Haidong Li

Ming Zhang (National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences); Haidong Li (National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences); Hongchuang Li (National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences); Xiuchao Zhao (National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences); Xiaoling Liu (National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences); Yeqing Han (National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences); Xianping Sun (National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences); Chaohui Ye (National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences); Xin Lou (Department of Radiology, Chinese PLA General Hospital); Xin Zhou (Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences)

Stroke is the second leading cause of death worldwide. 1H MRI has been increasingly used in the diagnosis and management of acute stroke. However, 1H MRI has a large background signal from biological tissue. Here, we demonstrated the feasibility of isotropic 3D high-resolution hyperpolarized 129Xe brain MRI and its potential for assessing the perfusion abnormalities caused by stroke. Permanent middle cerebral artery occlusion (MCAO) was performed on the rat, then 129Xe and 1H MRI were performed in sequence. Finally, a 3D high spatial-resolution129Xe brain image was obtained within 5 min, and hypoperfused areas observed with 1H and 129Xe images were well-matched. These results indicate that 3D 129Xe brain MRI is a promising method for stroke diagnosis.

11:30-11:50 **Using HP 129Xe MRI to Validate Proteomics Biomarkers in Early Cystic Fibrosis Lung Disease**

Presenting Author: Zackary Cleveland

Zackary Cleveland (Cincinnati Children's Hospital Medical Center); Abdullah S. Bdaiwi (Cincinnati Children's Hospital Medical Center); Matthew Siefert (Cincinnati Children's Hospital Medical Center); Emily Skala (Cincinnati Children's Hospital Medical Center); Assem G. Ziady (Cincinnati Children's Hospital Medical Center)

Cystic fibrosis (CF) is a progressive, historically fatal disease that has seen lifespans increase significantly due to improved therapies. However, these improvements have created a "victim of success" situation, where standard-of-care tools to can no longer monitor lung disease severity in many patients. Hyperpolarized (HP) 129Xe MRI can detect impaired ventilation years before changes the standard clinical tool—spirometry—but it is limited to a handful of specialize academic medical centers. Proteomic biomarkers from high-precision mass spectrometry can accurately forecast CF lung disease progression, but these biomarkers have only been validated in patients with spirometrically detectable lung disease. Here we use HP 129Xe MRI to validate proteomic markers in early severity and progression in CF lung disease.

MONDAY, APRIL 17, 2023 - *continued*

11:50-12:10 **The Effect of Elimination of Systematic Errors on the Distributions of Diffusion Tensor Imaging Metrics in Automatically Segmented Regions of White and Grey Matter of The Left and Right Hemisphere**

Presenting Author: Weronika Mazur

Weronika Mazur (AGH University of Science and Technology); Julia Lasek (AGH University of Science and Technology); Artur Krzyak (AGH University)

Neurodiseases can be assessed by diffusion tensor imaging (DTI) metrics in certain white (WM) and grey matter(GM) structures. In this study, we examined how the elimination of systematic errors (by using B-matrix spatial distribution, BSD) and enhancing SNR (by increasing number of excitations from 4, to 16 and 64, called NEX4, NEX16 and NEX64, respectively) change the distributions of mean diffusivity (MD) and fractional anisotropy (FA) in 95 automatically segmented WM and GM regions applying deep learning algorithm depending on the b-value. Results showed that without BSD application, systematic errors can cause artificial asymmetry between MD and FA values in the right and left hemisphere and GM and WM. b-value=2000 s/mm2 introduces strong kurtosis and skewness eliminated by BSD.

12:10-12:30 **Accurate Tomographic Magnetic Resonance T1 Mapping at Ultra-low Field**

Presenting Author: Sheng Shen

Sheng Shen (1. A. A. Martinos Center for Biomedical Imaging, Department of Radiology, MGH, 2.Harvard Medical School); Neha Koonjoo (1. A. A. Martinos Center for Biomedical Imaging, Department of Radiology, MGH, 2.Harvard Medical School); Stephen E. Ogier (1.University of Colorado, 2. National Institute of Standards and Technology); Kalina V. Jordanova (National Institute of Standards and Technology); Kathryn E. Keenan (National Institute of Standards and Technology); Matthew S. Rosen (1. A. A. Martinos Center for Biomedical Imaging, Department of Radiology, MGH, 2.Harvard Medical School, 3. Dept. of Physics, Harvard University)

Motivated by the growing contemporary interest in low field (<100 mT) and ultra-low field (<10 mT) MRI scanners, we have developed an accurate T1 mapping approach for use at ultra-low field that maintains its accuracy even in the low signal-to-noise ratio (SNR) regime at 6.5 mT. We describe here the use of a variable flip angle (VFA) method combined with accurate B1 correction. A hybrid B1 mapping method was used to increase the accuracy of low flip angle maps and thus increase the accuracy of T1 maps. We validated that our T1 mapping approach in a human tissue-mimic phantom has a deviation lower than 10% when compared to the ground truth obtained using an inversion recovery (IR) spectroscopic method.

MOF: Small Molecules: Emerging Methods and Applications (parallel session)
10:45-12:35, Nautilus

10:45-11:10 **Insights into Fluorinated Drug Substance and Drug Product via 19F Solid-State NMR Spectroscopy**

Presenting Author: Joe Lubach

Joe Lubach (Genentech, Inc.)

High resolution characterization of pharmaceutical solid dosage forms represents an ever-challenging and ever-changing problem facing pharmaceutical scientists. 19F solid-state NMR is becoming increasingly utilized around the community due to its sensitivity, exquisite selectivity, and prevalence in modern drug candidates. We will examine a few of the advantages, and drawbacks, of 19F solid-state NMR, and a variety of ways it can be exploited in solid form analysis. These include simple crystal form identification, crystallographic inequivalency evaluation, water content determination, and quantitative solid form measurements in complex drug products. Deeper understanding of drug particles in the presence of an excipient matrix offered by fluorine NMR can provide valuable insight into dosage form design for more robust drug products and processes.

11:10-11:30 **SHARPER-DOSY: Sensitivity Enhanced Diffusion-Ordered NMR Spectroscopy**

Presenting Author: Dusan Uhrin

George Peat (University of Edinburgh); Patrick J. Boaler (University of Edinburgh); Claire L. Dickson (Oxford Instruments); Guy C. Lloyd-Jones (University of Edinburgh); Dusan Uhrin (University of Edinburgh)

A liquid-state NMR method, which increases the sensitivity of the existing techniques for the measurement of diffusion coefficients of pure compounds by a factor of 10-100, is reported. The associated 10²-10⁴-fold time saving is achieved by removing the chemical shift separation and splittings due to J couplings. Diffusion coefficients are measured from a narrow singlet (which is invariant to magnetic field inhomogeneity) obtained by signal acquisition embedded within short spin-echoes. The proposed experiment incorporates solvent suppression and signal selection. Using high field cryoprobe NMR spectrometers, SHARPER-DOSY makes it possible to measure in a matter of minutes diffusion coefficient of medium-size organic molecules using as little as few hundred nanograms of material.

MONDAY, APRIL 17, 2023 - *continued*

11:30-11:50 **Long-lived states in achiral aliphatic chains**

Presenting Author: Geoffrey Bodenhausen

Kirill Sheberstov (ENS); Anna Sonnefeld (ENS); Geoffrey Bodenhausen (ENS)

Long-lived states involving typically four protons of neighbouring CH2 groups in achiral aliphatic chains can be excited by selective irradiation at one or several frequencies. Such experiments open interesting perspectives of delocalised long-lived states that are relatively insensitive to paramagnetic relation agents, can be boosted by hyperpolarization, generalised to mixtures for drug screening, and be unravelled by chemical shift MRI methods.

11:50-12:10 **Barriers to Proton Resolution in Solids**

Presenting Author: Daria Torodii

Daria Torodii (EPFL); Pinelopi Moutzouri (EPFL); Bruno Simes De Almeida (EPFL); Lyndon Emsley (EPFL)

We address experimentally the factors that limit proton linewidths in ultrafast MAS solid-state NMR experiments, which include residual dipolar coupling, anisotropic bulk magnetic susceptibility (ABMS), and distributions of chemical shifts. We find that in many organic solids the dipolar contributions account for about 20-40% of the 1H linewidth at 100 kHz MAS and can be reduced or removed by faster MAS or pure isotropic approaches. The remaining 60-80% of the linewidth is dominated by inhomogeneous interactions including ABMS and chemical shift distributions which are explored by dilution, deuteration and two-dimensional 1H-1H correlation experiments at 100 kHz MAS. Our findings open up a series of new pathways to ultra-high resolution 1H NMR in solids.

12:10-12:35 **Fast prediction of solution-state NMR parameters across a wide 3D chemical space**

Presenting Author: Craig Butts

Ben Honore (University of Bristol); Calvin Yiu (University of Bristol)

We present our next generation machine learning system, IMPRESSION-G2, capable of predicting isotropic and anisotropic NMR parameters. It achieves accuracies comparable to the best quantum chemical methods, but can complete predictions in milliseconds per molecule rather than hours or days. Crucially it accounts for stereochemical and conformational effects, making rapid 3D structure elucidation and verification practical and robust.

ASILOMAR LODGER LUNCH for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees may purchase a lunch ticket bundle or dinner ticket online by April 7.
12:45-14:00, Crocker Dinning Hall

POSTER SESSION with Exhibit Booths
14:00-15:45, Fireside Pavilion
See Poster Listings at end of document.

MOG: BioSolution: Condensed or Cellular (parallel session)
16:00-17:50, Merrill Hall

16:00-16:25 **Quenched H/D exchange NMR of inclusion bodies reveals significant native-like protein structure**

Presenting Author: Elizabeth Meiering

Elizabeth Meiering (University of Waterloo)

Protein aggregation is at the nexus of molecular processes crucial to aging, disease, and employing proteins for biotechnological and medical applications. While there has been considerable recent progress in determining structural features of protein aggregates formed in cells, owing to prevalent heterogeneity in aggregation, many aspects remain obscure. We report high-resolution analysis by quenched amide hydrogen/deuterium exchange NMR and complementary methods of cellular inclusion body aggregates for ALS-associated mutants of superoxide dismutase, engineered target binding proteins known as Adnectins or monobodies, and myoglobin. In contrast to prior studies reporting prominent amyloid in inclusion bodies, we find evidence for significant native-like structure. The results indicate an ensemble of protein self-association processes may contribute to IB formation.

MONDAY, APRIL 17, 2023 - *continued*

16:25-16:45 **Real-Time NMR Multiplexed GEF Assay Allowing the Monitoring of Multiple sGTPases Nucleotide Exchange from Cells and Organoids, Simultaneously**

Presenting Author: Genevieve Seabrook

Genevieve Seabrook (University Health Network-Princess Margaret Hospital); Teklab Gebregiworgis (Department of Biochemistry); Christopher B. Marshall (University Health Network-Princess Margaret Hospital); Tadateru Nishikawa (JEOL); Nikolina Radulovich (University Health Network-Princess Margaret Hospital); Ming Tsao (University Health Network-Princess Margaret Hospital); Mitsuhiko Ikura (University Health Network-Princess Margaret Hospital)

Small GTPases are regulators mediating important cellular functions. These sGTPases are often mutated in human cancers. We have developed a real-time multiplex NMR assay allowing the following of several sGTPases nucleotide exchange in a single experiment. Along with sGTPase proteins strategically selectively labeled, time-shared NMR methodology was used to reduce acquisition time. Analysis of sGTPases amides chemical shift changes, allowed us to identify residues that have been perturbed during the nucleotide exchange and the resulting structural changes within the sGTPases. A mixture of six sGTPases was used to assay GEF activities present in cells lysates and in organoids lysates. A combination of selective isotopic labeling and real-time, time-shared NMR experiments can be extended to other biological processes.

16:45-17:05 **Decoupling Protein Concentration and Aggregate Content Using Diffusion and Water NMR**

Presenting Author: Mark I. Grimes

Mark Grimes (University of Cambridge); Matthew Cheeks (AstraZeneca); Jennifer Smith (AstraZeneca); Fabio Zurlo (AstraZeneca); Mick D. Mantle (University of Cambridge)

Water proton nuclear magnetic resonance (wNMR) utilises the water transverse relaxation rate [$R_2(^1H_2O)$] to gain understanding about solutes. It has been used in this manner to obtain information about solution protein concentration and aggregate content, under both static and flow conditions. However, $R_2(^1H_2O)$ is influenced by both characteristics, so is unable to differentiate between them. In this work, the water diffusion coefficient [$D(^1H_2O)$] is used in conjunction with $R_2(^1H_2O)$ to separate these values. It has been demonstrated using three different model protein systems, in concentration ranges relevant for the maximum antibody titres found in fed batch bioreactors. This method allows for the rapid and facile determination of both protein concentration and aggregate content in a non-invasive manner.

17:05-17:25 **Long-lived Spin Order for Magnetization Transport: Overhauser Transfer and Stroboscopic Follow-up of Redox Reactions**

Presenting Author: Paul Vasos

Paul Vasos (ELI-NP/IFIN-HH); Florin Teleanu (ELI-NP/IFIN-HH); Adonis Lupulescu (ELI-NP/IFIN-HH); Adrian M. Voda (ELI-NP/IFIN-HH); Aude Sadet (ELI-NP/IFIN-HH)

Long-lived coherences (LLC's) and long-lived states (LLS) extend available timescales for magnetization transfer. Rotating-frame Overhauser transfer can be enhanced using LLC configurations. We measured LLC-ROE transfer between Ala-Hα and Gly-Hα1,2 in AlaGly. LLC-ROE transfer becomes more intense than via classical ROE for molecular rotational correlation times τc > 10 ns. LLC-ROE applications will be discussed for different symmetry configurations in peptides and for protein Lysozyme. Stroboscopic LLS is introduced for on-the-fly detection of molecular transformations on time-scales of tens of seconds. This is demonstrated for the follow-up of glutathione GSH/GSSG redox conversion starting from the initial polarization of GSH-Gly-Hα1,2, where lifetimes T_LLS of 16 s are reached. The stroboscopic LLS method is adapted for use with dissolution-DNP enhanced magnetization.

17:25-17:50 **Combining Laser and NMR for the Surface Analysis of Intrinsically Disordered Proteins**

Presenting Author: Jung Ho Lee

Jung Ho Lee (Seoul National University)

We present a photo-chemically induced dynamic nuclear polarization (photo-CIDNP) experiment suitable for the analysis of intrinsically disordered proteins (IDPs). Pulse stretching of laser pulses, band-selective decoupling of 13Cα, and simultaneous application of radiofrequency and laser pulses were implemented to quantitatively analyze the IDP surface at ultrahigh resolution. Comparative analysis with other surface accessibility methods validated the newly developed method and emphasized the importance of dye charge. Using the neutral riboflavin dye, surface accessibilities were measured to be nearly identical throughout the alpha-synuclein sequence. Divalent cations were shown to induce compaction of the C-terminal region and release of the N-terminal region of alpha-synuclein. This new method can be used as an orthogonal and independent method for investigating the overall IDP conformation.

MONDAY, APRIL 17, 2023 - *continued*

MOH: BioSolids I (parallel session)
16:00-17:45, Chapel

16:00-16:25 **Oxygen-17 NMR Studies of Proteins: Opportunities and Challenges**

Presenting Author: Zhehong Gan

Gang Wu (Queen's University)

One of the long-standing challenges in 17O NMR studies of proteins is the production of site-specifically or uniformly 17O-labeled proteins [1]. Recently, we demonstrated that it is feasible to achieve amino acid-type specific 17O-labeling of proteins via recombinant expression in an auxotrophic Escherichia coli strain [2]. This new approach allows incorporation of 17O isotopes into both the protein backbone and side chains. This opens up new opportunities for 17O NMR studies of proteins. In this talk, we will discuss this new 17O-labeling approach and present new 17O NMR data obtained with the latest NMR technologies including the uses of an ultra-high magnetic field (35.2 T) and a CryoProbe.

[1] G. Wu, Prog. Nucl. Magn. Reson. Spectrosco. 114/115, 135 (2019).

[2] B. Lin, I. Hung, Z. Gan, P.-H. Chien, H. L. Spencer, S. P. Smith, and G. Wu, ChemBioChem 22, 826 (2021).

16:25-16:45 **Biomolecular MAS NMR: some good reasons for spinning faster**

Presenting Author: Zhiyu Sun

Zhiyu Jeff Sun (Centre de Rsonance Magntique Nuclaire Trs Hauts Champs, Institut des Sciences Analytiques (UMR 5280 CNRS, Ecole Normale Suprieure de Lyon, Universit Claude Bernard Lyon 1), Universit de Lyon, 69100 Villeurbanne, France); Tanguy Le Marchand (Centre de Rsonance Magntique Nuclaire Trs Hauts Champs, Institut des Sciences Analytiques (UMR 5280 CNRS, Ecole Normale Suprieure de Lyon, Universit Claude Bernard Lyon 1), Universit de Lyon, 69100 Villeurbanne, France); Claire Ollier (Centre de Rsonance Magntique Nuclaire Trs Hauts Champs, Institut des Sciences Analytiques (UMR 5280 CNRS, Ecole Normale Suprieure de Lyon, Universit Claude Bernard Lyon 1), Universit de Lyon, 69100 Villeurbanne, France); Kumar Tekwani Movellan (Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716, USA; Pittsburgh Center for HIV Protein Interactions, University of Pittsburgh, Pittsburgh, PA 15260, USA); Brent Runge (Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716, USA; Pittsburgh Center for HIV Protein Interactions, University of Pittsburgh, Pittsburgh, PA 15260, USA); Kristof Grohe (Bruker BioSpin); Jochem Struppe (Bruker BioSpin); Sebastian Wegner (Bruker BioSpin); Angela Gronenborn (Department of Structural Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA, 15261, USA); Tatyana Polenova (Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716, USA; Pittsburgh Center for HIV Protein Interactions, University of Pittsburgh, Pittsburgh, PA 15260, USA); Guido Pintacuda (Centre de Rsonance Magntique Nuclaire Trs Hauts Champs, Institut des Sciences Analytiques (UMR 5280 CNRS, Ecole Normale Suprieure de Lyon, Universit Claude Bernard Lyon 1), Universit de Lyon, 69100 Villeurbanne, France)

The switch from the traditional MAS NMR approaches with 13C and 15N detection to 1H has accelerated the site-specific analysis of complex immobilized biological systems and opened the way to samples of higher molecular weight and only available in limited amounts.

We will take the moves from a critical analysis of recent literature data, share our first results on a prototypical Bruker 0.4 mm probe capable of rates exceeding 150 kHz and discuss the expected impact of fast MAS on resolution and sensitivity of NMR experiments on different classes of biomolecular samples.

16:45-17:05 **1H-31P Cross Polarization in White Matter Tissue: Towards New Contrast Mechanisms for MRI and Beyond!**

Presenting Author: Cariad-Arianna Knight

Cariad Knight (University of British Columbia); Alex Ensworth (University of British Columbia); Carl Michal (UBC)

MRI is in dire need of better myelin characterization tools. We present the use of solid-state NMR techniques to investigate myelin bilayers through direct detection of phospholipid phosphorous (31P) via dipolar coupled protons (1H) by cross polarization (CP), magnetization transfer (MT), and a hybrid MT-CP sequence. Results from porcine white matter indicate that CP provides a highly effective and specific myelin solid 31P filter in both static and magic angle spinning experiments. MT-CP experiments demonstrate magnetization exchanged between solid and aqueous 1H is detectable in subsequent 31P CP spectra. Additional experiments including wideline separation, spin echo double resonance and relaxation measurements provide further insight to myelin lipid health. This work enthusiastically supports development of a CP-based MRI contrast mechanism.

MONDAY, APRIL 17, 2023 - *continued*

17:05-17:25 **Structure and Dynamics of Microtubule- and Membrane-Bound Tau Protein from Solid-State NMR**

Presenting Author: Nadia El Mammeri

Nadia El Mammeri (MIT); Aurelio J. Dregni (MIT); Pu Duan (MIT); Olivia Gampp (MIT); Mei Hong (MIT)

The intrinsically disordered protein tau associates with and stabilizes microtubules to maintain neuronal health. Tau is also thought to interact with lipid membranes, which may play a role in the propagation of neurofibrillary tangles in Alzheimer's disease (AD). To understand the mechanism of the early misfolding events in AD, we have used magic-angle-spinning ssNMR to investigate the structure and dynamics of tau bound to microtubules and lipid bilayers. We present a new paradigm of tau's microtubule binding properties, and we reveal interesting mechanistic insights from membrane-induced tau amyloid fibrils. These results have important implications for the functional and pathological states of tau in diseases and demonstrate the power of solid-state NMR to investigate complex biomolecular assemblies in neurodegenerative diseases.

17:25-17:45 **High-Resolution 17O Solid-State Nuclear Magnetic Resonance of Peptides: 1H Detected HCO and HNO MQMAS**

Presenting Author: Zhehong Gan

Ivan Hung (Florida State University); Eric G. Keeler (New York Structural Biology Center); Wenping Mao (NHMFL, Florida State University); Peter Gorkov (NHMFL, Florida State University); Robert Griffin (Massachusetts Institute of Technology); Zhehong Gan (NHMFL, Florida State University)

Oxygen is an integral component of proteins but remains sparsely studied because its only NMR active isotope, 17O, has low sensitivity, low resolution, and large quadrupolar couplings. These issues are addressed here with efficient isotopic labeling, high magnetic fields, fast sample spinning, and 1H detection in conjunction with multidimensional experiments to observe oxygen sites specific to each amino acid residue. Sequential assignments and long-range distance restraints are demonstrated by using 3D 1H/13C/17O and 1H/15N/17O experiments, suggesting that such methods can become an essential tool for biomolecular structure determination. The use of 17O for initial polarization is found to provide better sensitivity per unit time compared to 1H.

MOI: Inorganic and Hybrid Materials (parallel session)
16:00-17:50, Nautilus

16:00-16:25 **Octahedral Tilt Engineering: Atomic-Level Picture of Stabilized α-FAPbI3**

Presenting Author: Dominik J. Kubicki

Tiarnan A. S. Doherty (Cavendish Laboratory, University of Cambridge,); Satyawan Nagane (Cavendish Laboratory, University of Cambridge,); Dominik Kubicki (University of Warwick); Young-Kwang Jung (Department of Materials Science and Engineering, Yonsei University); Duncan N. Johnstone (Department of Materials Science and Metallurgy, University of Cambridge); Affan N. Iqbal (Cavendish Laboratory, University of Cambridge); Dengyang Guo (Cavendish Laboratory, University of Cambridge); Kyle Frohna (Cavendish Laboratory, University of Cambridge); Mohsen Danaie (Electron Physical Science Imaging Centre, Diamond Light Source Ltd.); Elizabeth Tennyson (Cavendish Laboratory, University of Cambridge); Stuart Macpherson (Cavendish Laboratory, University of Cambridge); Anna Abfalterer (Cavendish Laboratory, University of Cambridge); Miguel Anaya (Cavendish Laboratory, University of Cambridge); Yu-Hsien Chiang (Cavendish Laboratory, University of Cambridge); Philip Crout (Department of Materials Science and Metallurgy, University of Cambridge); Simone Ruggeri (Laboratories of Organic and Physical Chemistry, Wageningen University and Research); Sean M. Collins (School of Chemical and Process Engineering and School of Chemistry, University of Leeds); Clare P. Grey (Yusuf Hamied Department of Chemistry, University of Cambridge); Aron Walsh (Department of Materials, Imperial College London); Paul A. Midgley (Department of Materials Science and Metallurgy, University of Cambridge); Samuel D. Stranks (Cavendish Laboratory, University of Cambridge)

Metal halide perovskites are used in optoelectronics research across the board and determining their atomic-level structure has been a growing area of solid-state NMR research over the past 5 years. I will give an overview of the recent progress, challenges and future directions in this area. I will focus particularly on the ternary formamidinium lead iodide as this material has excellent optical characteristics but is thermodynamically unstable and much of the current effort focuses on stabilizing its photoactive phase. We have developed a new stabilization strategy which relies on surface templating and results in remarkable phase stability. Solid-state NMR, NQR and scanning electron diffraction were key to understanding the atomic-level mechanism of this approach.

MONDAY, APRIL 17, 2023 - *continued*

16:25-16:45 **Migrating Solvation Structures in Li-ion Battery Electrolytes Revealed by Electrophoretic NMR**

Presenting Author: David Halat

David Halat (UC Berkeley & LBNL); Julia Im (University of California, Berkeley); Chao Fang (University of California, Berkeley); Aashutosh Mistry (Argonne National Laboratory); Saheli Chakraborty (University of California, Berkeley); Darby Hickson (University of California, Berkeley); Venkat Srinivasan (Argonne National Laboratory); Rui Wang (University of California, Berkeley); Nitash Balsara (University of California, Berkeley); Jeffrey Reimer (University of California, Berkeley)

The rapid (dis)charge capability of Li-ion batteries, an important metric for electric vehicle adoption, strongly depends on relative transport of ions and solvent within the electrolytic phase. Electrophoretic NMR (eNMR), wherein PFG experiments are synchronized with an applied electric field, can directly quantify the direction and magnitude of cation (⁷Li), anion (¹⁹F), and solvent (¹H) motion with spectroscopic specificity in Li-ion battery electrolytes. We report ¹H eNMR measurements of solvent velocity in model LiTFSI/tetraglyme electrolytes that reveal cation–solvent coordination, complementing molecular dynamics (MD) snapshots depicting specific cationic solvation structures. We also extend eNMR measurements to multivalent systems, i.e., polyanionic electrolytes, where we measure negative cation velocities that suggest Li⁺ moves the "wrong way" under electric field application.

16:45-17:05 **Probing the Local Environments of Cu(I) in Metal-Organic Frameworks via 63/65Cu Solid-state NMR Spectroscopy**

Presenting Author: Wanli Zhang

WANLI ZHANG (Western University); Bryan E.G. Lucier (Western University); Victor V. Terskikh (National Research Council Canada); Yining Huang (Western University)

For the first time, a series of Cu(I)-containing metal-organic framework (MOFs) with Cu sites in different coordination environments have been examined by using 63/65Cu wide-line NMR at 21.1 T. The 63/65Cu wide-line spectra were successfully acquired by Hahn-echo/WURST-CPMG sequences combined with VOCS (variable-offset cumulative spectra) method. The diversity of local environments of Cu(I) centers leads to a wide range of the quadrupolar coupling constant, ranging from 18.8 to 74.8 MHz depending on the Cu(I) local geometry. The NMR parameters were calculated by using plane-wave DFT calculations to aid the structural refinements of MOF systems. We demonstrate that the combination of 63/65Cu solid-state NMR and theoretical calculations can provide valuable structure information on local environment of copper metal ions/clusters within MOFs.

17:05-17:25 **Decoding the Microscopic Structure and Dynamics in Honeycomb-layered Sodium-ion Conductors: Na2MgxZn2-xTeO6 (x = 0 – 2) Using Solid-state NMR Spectroscopy**

Presenting Author: Diganta Sarkar

Diganta Sarkar (University of Alberta); Amit Bhattacharya (University of Alberta); Vladimir K. Michaelis (University of Alberta)

Sodium-ion batteries are emerging as a prospective alternative to lithium-ion batteries by offering low cost, improved safety, and superior sustainability. Solid-state NMR spectroscopy can provide a robust understanding of atomic-level structure and local Na-ion conduction to achieve their enhanced bulk performance. Here, we discuss a solid-state NMR method for comprehensive structure-property characterization of the honeycomb-layered solid electrolytes, Na2MgxZn2-xTeO6 ($0 \leq x \leq 2$), complemented by powder X-ray diffraction. The progression of Zn/Mg mixing in honeycomb layers and the influence of Zn/Mg order/disorder on bulk activation energies will be featured in this presentation. Furthermore, we study the variable-temperature 23Na spin-lattice relaxation to probe local Na-ion migration energies, and to determine how certain compositions may influence local Na-ion dynamics.

MONDAY, APRIL 17, 2023 - *continued*

17:25-17:50 **Combination of 17O NMR and computational modelling for the characterization of structure and dynamics in various systems containing COO groups**

Presenting Author: Christel Gervais

Christel GERVAIS (LCMCP - Sorbonne Universite); christian bonhomme (Sorbonne University); Hung Ivan (National High Magnetic Laboratory); Zhehong Gan (National High Magnetic Laboratory); Vinicius Martins (The University of Western Ontario); Bryan Lucier (The University of Western Ontario); Yining Huang (The University of Western Ontario); Jun Xu (National Institute for Advanced Materials, Nankai University); Thomas-Xavier Metro (IBMM, Universite de Montpellier); Cesar Leroy (ICGM, Universite de Montpellier); Ieva Goldberga (ICGM, Universite de Montpellier); Jessica packova (ICGM,Universite de Montpellier); Chia-Hsin Chen (ICGM, Universite de Montpellier); Danielle Laurencin (CNRS)

17O NMR spectroscopy is a very interesting characterization technique since oxygen can exhibit a wide variety of bonding in many molecules and materials. Thanks to selective 17O-enrichment, high-resolution 17O ssNMR spectra can be recorded and interpreted thanks to the use of DFT calculations : this combined experimental/theoretical approach allows a precise positioning of hydrogens and the nature of the H-bonding network to be established as well as binding modes of ligands. This will be illustrated in various systems including Zn and Al-based MOFs. In addition to the validation of structural models, 17O NMR data can also help to probe local dynamics as observed for instance in ibuprofen. Motions related to carboxylic groups were investigated with the help of computationnal modeling.

ASILOMAR LODGER DINNER for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees may purchase a lunch ticket bundle or dinner ticket online by April 7.
18:00 – 19:00, Crocker Dinning Hall

Vendor Hospitality Suites
From 19:00 onward

AMMRL Meeting
19:00-20:30, Chapel

TUESDAY, APRIL 18, 2023

Early Morning Lecture Series (for Students & ALL who wish to learn!)
07:00-07:50, Merrill Hall

07:00-07:50 **Understanding NMR Spectroscopy** Part 2 of 4

Presenter: James Keeler

Would you like to deepen or brush up your understanding of NMR theory? Join us for a morning lecture series by **James Keeler** (University of Cambridge), author of *Understanding NMR Spectroscopy*. These lectures assume only a modest prior knowledge of NMR theory and will cover some key topics of wide interest to budding NMR spectroscopists. Topics will include: Energy levels, Hamiltonians and operators; Introducing and using product operators; Relaxation; Coherence selection by phase cycling and field gradients

ASILOMAR LODGER BREAKFAST for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees cannot purchase breakfast tickets, but you can purchase lunch and dinner tickets by April 7.
07:30-09:00, Crocker Dining Hall

TOA: BioSolids II (parallel session)
8:45 - 10:10, Merrill Hall

08:45-09:10 **The Mechanisms of Lipid-targeting Antibiotics**

Presenting Author: Markus Weingarth

Markus Weingarth (Utrecht University)

Antimicrobial resistance is a global health threat, calling for new antibiotics. Good candidates could be compounds that target special lipids that only exist in bacterial, but not in human cell membranes. These drugs kill pathogens without detectable resistance. This has generated huge interest.

Using ssNMR and microscopy, our group has introduced approaches to study lipid-targeting antibiotics at different length-scales in membranes(1,2). Recently, we determined the killing mechanism of teixobactin(3), considered the first new antibiotic in 30 years. We showed that teixobactin kills bacteria by forming supramolecular fibrils that compromises the bacterial membrane. In addition, we show the mechanism of Clovibactin, a new antibiotic from 'unculturable' bacteria.

1. Medeiros-Silva, Nature Communications (2018)

3. Shukla, Nature Communications (2020)

2. Shukla, Nature (2022)

09:10-09:30 **NMR Crystallography of Tyrosine Phenol Lyase: Refining the Crystal Structure and Highlighting the Active Site Chemistry**

Presenting Author: Rittik K Ghosh

Rittik Ghosh (Department of Biochemistry, University of California - Riverside, CA 92521); Maria Luiza Caldas Nogueira (The University of Florida); Frederic M. Vigier (National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310); Joanna Long (University of Florida); Len Mueller (University of California Riverside)

We make use of an integrative combination of DNP enhanced solid-state NMR, X-ray crystallography, and first principles computational chemistry to solve for the atomic-resolution, three-dimensional structure of the active site for the quinonoid intermediate of tyrosine phenol lyase, a 206 kDa pyriodoxal-5'-phosphate dependent enzyme. Most importantly, this NMR crystallographic approach allows us to delineate the mechanistically significant protonation states that define the active site chemistry and reconcile inconsistencies between previous X-ray crystal structures. Our refined active site structure satisfies both the experimental chemical shift restraints and the active site electron density for the bound substrate, which was previously poorly fit by the reported structural model.

TUESDAY, APRIL 18, 2023 - *continued*

09:30-09:50 **Solid-state NMR analysis of the Pseudomonas aeruginosa biofilm matrix**

Presenting Author: Courtney Reichhardt

Courtney Reichhardt (Washington University)

Most bacteria live as multi-cellular communities termed biofilms, which protects bacteria against harsh conditions. Within biofilms, bacterial cells are entangled in a biopolymer-rich extracellular matrix that is rich in biopolymers. Previously, it was determined that up to three structurally distinct exopolysaccharides as well as several proteins and extracellular DNA contribute to Pseudomonas aeruginosa biofilm matrices. The presence of different exopolysaccharides in P. aeruginosa biofilm matrices results in varying viscoelastic properties of the biofilms, which is related to the virulence of the bacteria. We hypothesized that these viscoelastic properties arise due to different dynamics and interactions of exopolysaccharides within the biofilm matrix. To test this hypothesis, we used solid-state NMR to investigate the composition and dynamics of P. aeruginosa biofilm matrices.

09:50-10:10 **Magic-Angle Spinning NMR and Integrated Approaches for Structure Determination of Microtubule-Associated Proteins Assembled with Microtubules**

Presenting Author: Changmiao Guo

Changmiao Guo (Department of Chemistry and Biochemistry, University of Delaware); Chunting Zhang (Department of Chemistry and Biochemistry, University of Delaware); Raymundo Alfaro-Aco (Department of Molecular Biology, Princeton University); Ryan W. Russell (Department of Chemistry and Biochemistry, University of Delaware); Caitlin M. Quinn (Department of Chemistry and Biochemistry, University of Delaware); Mingyue Li (Department of Chemistry and Biochemistry, University of Delaware); Angela M. Gronenborn (Department of Structural Biology, University of Pittsburgh School of Medicine); Sabine Petry (Department of Molecular Biology, Princeton University); John C. Williams (Department of Molecular Medicine, Beckman Research Institute of City of Hope); Tatyana Polenova (Department of Chemistry and Biochemistry, University of Delaware)

We demonstrate magic-angle spinning (MAS) NMR and integrated approaches for structure elucidation of microtubule-associated proteins assembled with microtubules, including kinesin-1 motor domain (KIF5B) and active domain of a microtubule nucleation factor. We determined an all-atom NMR structure of KIF5B in complex with microtubules by integrating MAS NMR restraints with the medium-resolution cryo-EM density map. Additionally, we report the structure of the targeting protein for Xklp2 C-terminal domain involved in a condensate on microtubules using 1H-detected fast MAS NMR and molecular modeling. These studies provided atomically detailed insights unavailable from other methods, such as binding interfaces with microtubules, and "invisible" dynamically disordered regions of biological assemblies.

TOB: Instrumentation I (parallel session)
8:45 - 10:15, Chapel

08:45-09:10 **Silicon-chip based small NMR spectrometers**

Presenting Author: Donhee Ham

Donhee Harvard (Harvard University)

Over the past ca. 15 years, we have been developing miniaturized nuclear magnetic resonance (NMR) spectrometers by conflating small permanent magnets and silicon radio-frequency transceiver integrated circuits. They have been able to perform a diverse set of multi-dimensional NMR relaxometry and spectroscopy experiments, resolving J-coupled spectra for small molecules, and magnetic resonance imaging (MRI). These portable, affordable, and low-maintenance NMR spectrometers may enable in-field, on-demand, or online applications for small molecular fingerprinting, chemical reaction monitoring, biomolecular sensing, quality control, subsurface exploration, and imaging of ex vivo biological tissues as well as artificial organoids, small organisms, and organic material systems. In this presentation, I will review these small NMR platforms and their future perspectives.

09:10-09:30 **190 GHz Single Chip Dynamic Nuclear Polarization Microsystem**

Presenting Author: Nergiz Sahin Solmaz

Nergiz Sahin Solmaz (Ecole Polytechnique Federale de Lausanne); Reza Farsi (Ecole Polytechnique Federale de Lausanne); Giovanni Boero (Ecole Polytechnique Federale de Lausanne)

We report on a single chip DNP microsystem operating at 190 GHz. The ESR detector consists of a 190 GHz oscillator with oscillation amplitude detection. The frequency of the oscillator is tunable up to 5 GHz. The NMR detector is a receiver-only chain with 75 dB overall gain, consisting of a 10 turns microcoil with a diameter of about 200 um, a broadband LNA operating up to 1 GHz, a mixer, and a LF amplifier with 4 MHz bandwidth. An external coil is used for NMR excitation. At the conference, ESR, 1H NMR, and 1H DNP-NMR spectra acquired with solid samples at about 6.8 T at room temperature as well as at low temperature will be presented.

TUESDAY, APRIL 18, 2023 - *continued*

09:30-09:50 **A flexible low cost microchip-based NMR system for micro-scale applications**

Presenting Author: Kathryn Marable

Kathryn Marable (Annaida Technologies); Marco Grisi (Annaida Technologies SA); Guillaume Gruet (Annaida Technologies); Giulia Sivelli (Annaida Technologies); Gaurasundar Conley (Annaida Technologies)

Micro-NMR is a growing area within the field of NMR that allows increased sensitivity with reduced sample volume demands [1]. We present here a scalable micro-NMR, user-friendly, and broadband probe system. The probe can be used with standard NMR spectrometers in measurements of samples with volumes from 10 nL to 100 pL at frequencies between 150 MHz and 600 MHz. The use of additive manufacturing allows customization and adaptation for a wide range of magnets, spectrometer systems, and applications. Furthermore, the CMOS-based design allows for simultaneous acquisition from multiple sensor coils on the same device. This presentation discusses the system architecture, features, and performance, as well as prospects for future developments.

09:50-10:15 **Zero-dead-time detection and other advances in oscillator-based NMR and EPR**

Presenting Author: Jens Anders

Jens Anders (University of Stuttgart); Michal Kern (University of Stuttgart); Bernhard Bluemich (RWTH Aachen); Klaus-Peter Dinse (Helmholtz-Zentrum Berlin fuer Materialien und Energie); Klaus Lips (Helmholtz-Zentrum Berlin fuer Materialien und Energie)

In this invited talk, after a brief introduction to the working principle of VCO-based MR, including a detailed explanation of its ability for zero-deadtime-detection, we will present our latest research results in this field together with a discussion of the advantages and drawbacks of this method compared to classical MR detection. We will close the talk with a brief outlook on future research directions in VCO-based MR.

COFFEE BREAK with Exhibit Booths and Posters, Fireside Pavilion
10:20-10:45

TOD: Impacts of Metabolomics (parallel session)
10:45-12:30, Merrill Hall

10:45-11:10 **NMR and the Brazilian flora: a successful combination in the identification of Leishmania donovani nucleoside hydrolase inhibitors**

Presenting Author: Luzineide Wanderley Tinoco

Bruno Clemente B. Marques (Universidade Federal do Rio de Janeiro); Gregorio Torres Rangel (Universidade Federal do Rio de Janeiro); Guilherme S. Caleffi (Universidade Federal do Rio de Janeiro); Joao Avelar (Universidade Federal do Rio de Janeiro); Paulo Roberto Ribeiro Costa (Universidade Federal do Rio de Janeiro); Luzineide Tinoco (Universidade Federal do Rio de Janeiro)

Nucleoside hydrolases are a strategic target for drug development to treat leishmaniasis, a neglected disease. The identification of flavonoids as inhibitors of Leishmania donovani nucleoside hydrolase (LdNH) emerged from the biological screening of 214 extracts from Brazilian plants. Three plants were selected for their results and lack of previous phytochemical description: Leandra amplexicaulis, Urvillea rufescens, and Ormosia arborea. The use of NMR combined with chemometrics allowed the identification of two new proanthocyanidins as LdNH inhibitors before isolation, directing the best strategy to purify them. From this identification, a series of flavonoids was synthesized and their activities determined. STD and Waterlogsy data, obtained for the most potent flavonoids, combined with docking studies, provided information on structure-activity relationships.

11:10-11:30 **A New Limit for Blood Metabolite Analysis Using 1H NMR Spectroscopy**

Presenting Author: G. A. Nagana Gowda

G. A. Nagana Gowda (University of Washington); Vadim Pascua (University of Washington); Daniel Raftery (University of Washington)

The relatively small number of blood metabolites accessible by a simple 1D NMR method has restricted the scope of NMR applications in the metabolomics field. Enhancing the limit of identified metabolites in blood will therefore greatly impact NMR-based metabolomics. With a focus on addressing this challenge, and based on the comprehensive investigation of human blood and plasma using a combination of 1D/2D NMR techniques, we describe the identification of unknown metabolites and expanding the limits of quantifiable blood metabolites using NMR. The results provide access to nearly 90 metabolites, which is the highest to date for a simple 1D 1H NMR experiment that is widely used in the metabolomics field. The new findings are expected to greatly impact blood metabolomics.

TUESDAY, APRIL 18, 2023 - *continued*

11:30-11:50 **Mitochondrial Metabolism in Astrocytes is Essential for their Survival Against Neurotoxic Electrophile Exposure**

Presenting Author: Alexandra Crook

Alexandra Crook (University of Nebraska - Lincoln); Jordan Rose (University of Nebraska - Lincoln); Annadurai Anandhan (University of Nebraska - Lincoln); Christian Brian (University of Nebraska - Lincoln); Rodrigo Franco Cruz (University of Nebraska - Lincoln); Robert Powers (University of Nebraska - Lincoln)

Astrocytes regulate neuronal excitability and homeostasis, and they are the first line of defense against xenobiotics crossing into the brain. We demonstrate that astrocytes mitochondrial metabolism is essential for survival against neurotoxic electrophiles such as inorganic arsenic (iAs). Subtoxic iAs induced an increase in de novo GSH synthesis and a reduced intracellular environment in astrocytes. Targeted NMR metabolomics revealed that iAs induced the anaplerotic generation of glutamate via the TCA cycle, which contributes to GSH de novo synthesis. iAs exposure led to substantial extracellular glutamate accumulation that was mediated by reversal of the excitatory amino acid transporter 1. These results reveal that mitochondrial metabolism in astrocytes is required for the detoxification of neurotoxic electrophiles such as iAs.

11:50-12:10 **Pluronic F-127 as a gel matrix for in-cell NMR**

Presenting Author: Cale Thornton

Cale Thornton (Boise State University); Nicole Elizabeth Aughtry (Boise State University); Wesley Joseph Hirons (Boise State University); Lisa R. Warner (Boise State University)

In-cell NMR is a technique that can be used to analyze metabolic pathways in a wide variety of cells in vivo. However, cells larger than ~2 micrometers in diameter, tend to settle to the bottom of the NMR tube over the course of hours, no longer centered in the coil. This limits application of in-cell NMR to smaller cells, shorter experiment time, or specialty tubes. One approach to mitigate this problem is to suspend cells in a gelatinous medium. Pluronic F-127 is a biocompatible thermosensitive hydrogel that has potential as a gel matrix for in-cell NMR and has previously been used to study magnetically aligned Pf1 phage. Here, we examine Pluronic F-127 as a gel matrix for in-cell NMR experiments.

12:10-12:30 **Detection of Human Prostate Cancer using Multivoxel MR Spectroscopy Based Metabolomics Imaging**

Presenting Author: Leo Cheng

Leo Cheng (MGH Harvard Medical School)

Imaging detection of prostate cancer is still a challenging task in clinic. NMR-based metabolomics has demonstrated improved potential in disease diagnosis and characterization when compared with measurements of individual metabolites. Using a 7T human whole-body MRI system, we measured multivoxel MRS for 30 prostates removed from patients with biopsy-proven cancer. These 30 cases were divided into Training and Testing cohorts. Cancer discriminating canonical analysis was conducted on the Training cohort and applied to the Testing cohort. Metabolomics imaging profiles thus discovered demonstrate the superior capability when compared with parameters currently used in clinic. Although obtained from removed prostates, these results, measured on a whole-body MRI system, can be implemented directly in clinic, with its concept applicable to general clinical MR.

TOE: Simulations, Processing, and New Software (parallel session)
10:45-12:30, Chapel

10:45-11:10 **EasyNMR: Web-based data handling and NMR simulations**

Presenting Author: Thomas Vosegaard

Armin Afrough (Interdisciplinary Nanoscience Center, Aarhus University); Thomas Vosegaard (Interdisciplinary Nanoscience Center, Aarhus University)

We present a flow-based programming solution, EasyNMR, for numerical simulations in NMR and with a novel focus on cloud-based data storage and -sharing. With a web-based interface, EasyNMR needs no installation thus limiting the barrier for getting started yet maintains the versatility of more advanced NMR simulation software solutions.

TUESDAY, APRIL 18, 2023 - *continued*

11:10-11:30 **Spectroscopy as an inverse problem: Structure elucidation from 1D NMR spectral information via deep imitation learning**

Presenting Author: Eric Jonas

Eric Jonas (University of Chicago)

Small molecule structure elucidation has long been an area of active spectroscopic interest. Here we formulate structure elucidation as an inverse problem, akin to tomography or medical imaging, and develop new machine-learning techniques to elucidate small molecule structures entirely from shift data. We do this by leveraging an existing fast forward model (from structure to spectrum) and new graph-based machine learning methods. We can achieve 80% accuracy on structure recovery with carbon shifts and 40% accuracy with proton shifts. Additionally our method can produce quantified confidence estimates, saying when it "doesn't know" the correct solution for a given spectrum. We highlight future directions for this approach and quantify the overall identifiability of small molecule structures from shift spectra.

11:30-11:50 **Automated Large Scale 13-C & 1-H Chemical Shift Predictions of 40,000 Natural Products via DFT Calculations**

Presenting Author: Amy Jystad

Amy Jystad (Pacific Northwest National Laboratory); Jessica Bade (Pacific Northwest National Laboratory); Sean Colby (Pacific Northwest National Laboratory); John Cort (Pacific Northwest National Laboratory)

The gold standard for identification of novel natural products is structure elucidation by NMR spectroscopy. Unfortunately, most of this data is scattered in labs and print journals. This has spurred efforts to establish the Natural Products Magnetic Resonance Database (NP-MRD). NP-MRD is expected to contain ~350,000 structures, only a small portion (<15%) will likely have associated NMR data. To fill this gap, we are in the process of backfilling NP-MRD with DFT calculated NMR spectra. We have developed in silico Chemical Library Engine 2 (ISiCLE 2) to automate the prediction of chemical shifts, and Simulated NMR to Experiment Assignment Software LibrarY (SNEASY) to compare predicted and experimental shifts, resulting in the DFT chemical shift data of ~40,000 natural products.

11:50-12:10 **Rapid Prediction of Full Spin Systems using Uncertainty-Aware Machine Learning**

Presenting Author: Jake Williams

Jake Williams (University of Chicago); Eric Jonas (University of Chicago)

Accurate simulation of solution NMR spectra requires knowledge of all chemical shift and scalar coupling parameters. We present a novel machine learning technique which combines uncertainty-aware deep learning with rapid estimates of conformational geometries to generate Full Spin System Predictions with UnCertainty (FullSSPrUCe). We improve on previous state of the art in accuracy on chemical shift values, predicting protons to within 0.209 ppm and carbons to within 1.218 ppm. Further, we are able to predict all scalar coupling values, unlike previous GNN models, achieving 3JHH accuracies between 0.838-1.392 Hz on small experimental datasets. Uncertainty quantification shows a strong, useful correlation with accuracy, and we design a method to intelligently combine ab initio and experimental data.

12:10-12:30 **mrsimulator: A cross-platform object-oriented open-source software package for fast solid-state NMR spectral simulation and analysis**

Presenting Author: Philip Grandinetti

Deepansh Srivastava (Hyperfine, Inc); Matthew Giammar (Ohio State University); Lexi McCarthy (Ohio State University); Maxwell Venetos (University of California); Philip Grandinetti (Ohio State University)

The free and open-source Python package mrsimulator is a simple-to-use, easy-to-install, versatile library with a permissive license capable of simulating multi-dimensional solid-state NMR spectra of coupled spin systems under variable-angle spinning conditions. High simulation benchmarks are achieved using analytical solutions for transition frequencies and coherence transfers between transitions. This approach generalizes to multi-dimensional NMR spectra simulations using symmetry pathway concepts for describing multi-pulse NMR experiments. The efficiency gains with this approach are essential for the accurate spectral modeling of non-crystalline materials, where thousands of subspectra are needed for accurate line shape simulations. mrsimulator is fully documented with numerous examples (https://mrsimulator.readthedocs.io). It easily integrates with other scientific and machine-learning libraries to create new opportunities for data science with solid-state NMR spectroscopy.

TUESDAY, APRIL 18, 2023 - *continued*

ASILOMAR LODGER LUNCH for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees may purchase a lunch ticket bundle or dinner ticket online by April 7.
12:45-14:00, Crocker Dinning Hall

OR

UHF-NMR Lunch Meeting, RSVP by March 31
13:00-14:00

POSTER SESSION with Exhibit Booths
14:00-15:45, Fireside Pavilion
See Poster Listings at end of document.

TOG: Organic, Soft Matter and Biomaterials (parallel session)
16:00-17:45, Merrill Hall

16:00-16:25 **Developing models of extracellular matrix in health and ageing: NMR approaches**

Presenting Author: Melinda J Duer

Melinda Duer (University of Cambridge)

The extracellular matrix (ECM) forms the bulk of our structural tissues and provides them with their mechanical properties. Intriguingly, at the molecular level, the ECM provides the communication system between the cells and the signals that drive the individual behaviour of cells. Ultimately, if we can understand how the extracellular matrix molecular structure and dynamics dictates the behaviour of cells, then we can develop ways to combat the effects of ageing. However, understanding the molecular level properties of the extracellular matrix has been hampered by the lack of methods to study tissues at the atomic scale. In this talk, I will describe the NMR approaches that my group has taken and are continuing to develop to tackle these complex questions.

16:25-16:45 **Characterization of bound water in post-translationally modified amyloid-beta fibrils and a soil sample from Antarctica, using O-17 and H-2 NMR.**

Presenting Author: Liliya Vugmeyster

Liliya Vugmeyster (CU Denver); Dmitry Ostrovsky (CU Denver); Aryana Rodgers (CU Denver); Riqiang Fu (National High Magnetic Field Laboratory)

Water bound to interfaces of biological molecules or soils can have profound impact on functionality due to enhancement of motions and activation of interfaces. Using a combined approach with deuterium and oxygen-17 solid-state NMR, we present characterization of amounts and motions in bound water in two very distinct systems: amyloid-beta fibrils with a pyroglutamate post-translational modification and a soil sample from McMurdo Dry Valleys of Antarctica. Spectra, longitudinal and rotating frame relaxation times at two magnetic field strength values (18.8 and 9.4 T) and over a broad temperature range of 300 to 220 K provide means of obtaining amounts of free and bound water, as well as time scales of motions induced by interfacial interactions.

16:45-17:05 **Paramagnetic Guest Exchange Saturation Transfer (ParaGEST) Revealing Hidden Interactions in Supramolecular Host-Guest Systems**

Presenting Author: Elad Goren

Elad Goren (Mr.); Liat Avram (Dr.); Amnon Bar-Shir (Prof.)

The recently developed ¹⁹F-guest exchange saturation transfer (¹⁹F-GEST) approach adopts the principles of chemical exchange saturation transfer (CEST) for studying the binding kinetics of host-guest systems. Incorporating paramagnetic lanthanides to α- and β-cyclodextrins (creating Ln-α-CDs and Ln-β-CDs), to obtain ¹⁹F-paraGEST, allows to study faster exchange rates in NMR time scale.

Here we show that varying the pseudo-contact shift induced on an exchanging fluorinated guest provides insights into its dynamic interactions, not accessible by any other analytical tool. Specifically, benefiting from the enhanced spectral resolution of ¹⁹F-paraGEST, we could identify two different populations of a bound guest specific for Ln-β-CDs, implying different CD-binding geometries with similar activation energies. The results highlight the importance of ¹⁹F-paraGEST for studying "NMR-invisible" host-guest systems.

TUESDAY, APRIL 18, 2023 - *continued*

17:05-17:25 **Exploring Ion gating of conducting polymer PEDOT:PSS by Operando NMR Spectroscopy**

Presenting Author: Dongxun Lyu

Dongxun Lyu (University of Cambridge); Yanting Jin (University of Cambridge); Pieter Magusin (University of Cambridge); Evan Wenbo Zhao (University of Cambridge); Scott Keene (University of Cambridge); George Milliaras (University of Cambridge); Clare Grey (University of Cambridge)

The conducting polymer poly(3,4-ethylenedioxythiophene) poly(styrene sulfonate) (PEDOT:PSS) is regarded as the most promising organic mixed ionic-electronic conductors for applications in bioelectronics and energy storage. This has led to increasing interest in the development of new analytical methods to non-invasively visualise the transport and coupling of electronic and ionic charge carriers during device operation. Here we show that operando 1H and 23Na NMR spectroscopy can quantify cation and water movement during the doping/dedoping of PEDOT:PSS films. A distinct quadrupolar splitting is observed for sodium ions bound to anisotropic domains of the polymer films. Operando 23Na NMR studies reveal a close-to-linear correlation between the quadrupolar splitting and the charge stored in the film, which is quantitatively explained by a two-site exchange model.

17:25-17:45 **Decoupling the Effects of Thermal Cycling and Shear on Phase-Change Nano-Emulsions by NMR spectroscopy, Rheo-NMR, and MRI Velocimetry**

Presenting Author: Jungeun Park

Jungeun Park (The City College of New York); Ulrich Scheler (Leibniz Institute for Polymer Research); Robert J. Messinger (The City College of New York)

Organic phase-change material (PCM) nano-emulsions are formed by emulsifying oil in water in the presence of surfactant and can store or release thermal energy during phase transitions. However, PCMs nano-emulsions become unstable due to thermal cycling and shear in heat transfer systems. To better understand the molecular origins of these instabilities, liquid-state NMR measurements were applied to a model PCM nano-emulsion, enabling metastable supercooling effects to be monitored and revealing that the surfactant head group exists in multiple environments that change upon thermal cycling. 1H rheo-NMR and MRI velocimetry methods were also applied to measure the velocity profile and concentration distribution of oil within a Searle cell, revealing non-linear velocity profiles and shear-induced migration of the emulsion droplets.

TOH: BioSolution: Molecular Interactions and Energetics (parallel session)
16:00-17:45, Chapel

16:00-16:25 **The role of highly flexible regions in orchestrating the properties of multidomain proteins: insights from 13C detected NMR experiments**

Presenting Author: Isabella C Felli

Isabella Felli (University of Florence)

Highly flexible regions of complex multi-domain proteins introduce an additional dimension in protein function, still exploiting simple modules (globular domains and highly flexible regions themselves). This modular protein architecture is shared by many proteins involved in recognition, signaling and regulation, all processes in which structural and dynamic heterogeneity plays a fundamental role. Protein malfunction, linked to the onset of incurable diseases, is often related to highly flexible regions.

NMR represents a unique tool for their investigation at the atomic level. However when globular and disordered domains are simultaneously present in a protein, the NMR spectra can become quite complex. 13C detection offers an elegant approach to study them not only in isolation but also when part of complex multi-domain proteins.

16:25-16:45 **Quadruplex DNA Structures and Ligand Intercalation**

Presenting Author: Janez Plavec

Janez Plavec (National Institute of Chemistry)

DNA with its canonical duplex and alternative structures including quadruplex motifs are associated with many biological functions of DNA. NMR revealed structural details of four-stranded DNA architectures adopted by GGGAGCG repeats in the regulatory regions of genes responsible for neurological disorders. Their unique tetrahelical structures are distinctly different from G-quadruplexes. Complexes with bis-quinolinium ligand 360A exhibit intercalation between GAGA- and GCGC-quartets. On the other hand, Phen-DC3, one of the best-known G-quadruplex ligands causes dTAGGG(TTAGGG)3 to change its fold in KCl solution from a hybrid-1 to a chair-type structure, with the ligand intercalating between two G-quartets, ejecting a potassium ion. The unprecedented high-resolution NMR structure is the first to show true ligand intercalation into an intramolecular G-quadruplex.

TUESDAY, APRIL 18, 2023 - *continued*

16:45-17:05 **Pressure, Motion and Conformational Entropy in Molecular Recognition by Proteins**

Presenting Author: Josh Wand

Jose A. Caro (Texas A&M University); Kathleen G. Valentine (University of Pennsylvania); Taylor R. Cole (Texas A&M University); Josh Wand (Texas A&M University)

Molecular recognition is a determinant of biochemistry. A dynamic proxy using NMR-relaxation has revealed a richness in the contributions of conformational entropy (-TΔSconf) to binding thermodynamics. We examined the internal motion of barnase in a thermodynamic cycle over binding barstar and hydrostatic pressure. Motion in barnase, as evidenced by 15N and methyl deuterium relaxation, is conserved along the pressure-binding cycle. Binding has a -TΔSconf penalty of +11.7 kJ/mol at 1 bar. At 3kbar, the overall change in side chain motion (TΔSconf) is zero, suggesting a role for ΔSconf in the adaptation of proteins to extreme environments. Spatial clustering of the pressure sensitivity indicates that local contributions of ΔSconf can contribute to the thermodynamics of protein function.

17:05-17:25 **Investigation of the Allosteric Signaling Mechanism of a Thermostable GeoCas9 by Solution NMR**

Presenting Author: Helen Belato

Helen Belato (Brown University); George P. Lisi (Brown University)

CRISPR-Cas9 is a widely utilized biochemical tool. An understanding of the molecular motions that are critical for target DNA recognition, unwinding, and cleavage by Cas9 are unknown. In this study, we report an atomic level comparison of structural and dynamic properties of the Recognition lobe (Rec) and the HNH domain of a thermostable Cas9 (GeoCas9). We show that GeoHNH motions are regulated by fast (ps-ns) timescale dynamics. Furthermore, when the residue with the highest flexibility on the ps-ns timescale is mutated in GeoHNH, its protein solubility, thermal stability, and dynamic profile are drastically distorted. NMR studies of Rec show evidence of a contiguous millisecond timescale dynamic pathway throughout Rec, which links the adjacent GeoHNH domain for allosteric signaling.

17:25-17:45 **Modulation of co-translational protein folding on CRISPR/Cas9-engineered ribosomes investigated by solution NMR, cryoEM and MD simulations**

Presenting Author: Minkoo Ahn

Minkoo Ahn (University College London); Tomasz Wodarski (University College London); Alkistis Mitropoulou (University College London); Sammy Chan (University College London); Haneesh Sidhu (University College London); Elena Plessa (University College London); Thomas Becker (Ludwig-Maximilians-Universitt Mnchen); Nediljko Budisa (University of Manitoba); Christopher Waudby (University College London); Roland Beckmann (Ludwig-Maximilians-Universitt Mnchen); Anas Cassaignau (University College London); Lisa Cabrita (University College London); John Christodoulou (University College London)

To understand how co-translational protein folding is modulated by the narrow ribosome exit tunnel, we have rationally engineered three exit tunnel protein loops of the 70S ribosome by CRISPR/Cas9 gene editing, and studied the co-translational folding of an immunoglobulin-like filamin domain (FLN5). Our thermodynamics measurements employing 19F/15N/methyl-TROSY NMR spectroscopy reveal how the variations in the lengths of the loops (uL23, uL24) exert their distinct and concerted effects on the free energy of FLN5 folding and binding to the ribosome surface. This is highlighted by the opposite folding outcomes resulting from the loop extensions, and cryoEM and MD simulations show the structural basis of such changes, thereby providing principles for how to remodel them to elicit a desired folding outcome.

ASILOMAR LODGER DINNER for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees may purchase a lunch ticket bundle or dinner ticket online by April 7.
18:00 – 19:00, Crocker Dinning Hall

VENDOR HOSPITALITY SUITES
From 18:30

WEDNESDAY, APRIL 19, 2023

Early Morning Lecture Series (for Students & ALL who wish to learn!)
07:00-07:50, Merrill Hall

07:00-07:50 **Understanding NMR Spectroscopy** Part 3 of 4

Presenter: James Keeler

Would you like to deepen or brush up your understanding of NMR theory? Join us for a morning lecture series by **James Keeler** (University of Cambridge), author of *Understanding NMR Spectroscopy*. These lectures assume only a modest prior knowledge of NMR theory and will cover some key topics of wide interest to budding NMR spectroscopists. Topics will include: Energy levels, Hamiltonians and operators; Introducing and using product operators; Relaxation; Coherence selection by phase cycling and field gradients

ASILOMAR LODGER BREAKFAST for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees cannot purchase breakfast tickets, but you can purchase lunch and dinner tickets by April 7.
07:30-09:00, Crocker Dining Hall

WOA: Theoretical Treatment of Pulse Sequences and Experiments (parallel session)
8:45 - 10:10, Merrill Hall

08:45-09:10 **Pulse-Sequence Optimization Based on Effective Floquet Hamiltonians**

Presenting Author: Matthias Ernst

Matias Chavez (ETH Zurich); Matthias Ernst (ETH Zrich)

We present a new approach to pulse sequence optimization that is based on effective Floquet Hamiltonians and not state-to-state transfers using numerical simulations. Efforts to use effective Floquet Hamiltonians for pulse-sequence optimization have been hampered by the requirement to have a continuous transition from a resonant situation through a near-resonant and finally to a non-resonant effective Hamiltonian. Especially the near resonant case is difficult to describe using classical Floquet methods. We have introduced a frequency-continuous Floquet approach that allows us to obtain effective Hamiltonians in all three cases. Based on this approach, we will show first attempts to optimize pulse sequences for frequency-selective polarization transfer under MAS based on single-spin interaction-frame trajectories that can be calculated very efficiently.

09:10-09:30 **Low power optimal control pulses improve the performance of multidimensional Bio-molecular solution NMR experiments at ultrahigh-field 1.2 GHz (28.2 T) spectrometers**

Presenting Author: David Joseph

David Joseph (Max Planck Institute for Multidisciplinary Sciences, Gttingen, Germany); Christian Griesinger (Max Planck Institute for Multidisciplinary Sciences, Goettingen, Germany)

Bio-molecular NMR studies are usually limited by sensitivity and resolution, especially for concentration limited samples. At present, Bruker provides only a 3 mm CryoProbe for the 1.2 GHz spectrometers due to high power limitations. This restricts the study of concentration limited samples to a smaller sample volume. In this work, we have designed low power optimal control (OC) pulses for broadband universal rotation of 1H and 15N nuclei and introduce a new approach to designing OC band selective pulses. These pulses were utilized to construct low power 2D-OC-[1H,15N]-HSQC and 3D-OC-HNCO and their TROSY versions. These OC-sequences gave a performance improvement and we are confident that low power OC experiments can enable large volume measurements at the 1.2 GHz magnets.

09:30-09:50 **Towards more Robust Sparsity with Nonuniform Sampling in Challenging 2D NMR by Reducing Repeat Subsequences**

Presenting Author: Lucille E Cullen

Lucille Cullen (Bucknell University); Alan Marchiori (Bucknell University); David Rovnyak (Bucknell University)

Sampling noise and aliasing artefacts are a barrier to using sparser nonuniform sampling (NUS) in complex 2D NMR experiments. We find that weak aliasing artefacts are a growing concern in sparser 1D-NUS and can sometimes be misattributed to incomplete deconvolution of the broader point-spread function. As sparsity increases in NUS, we find that detrimental repeat sequences can occur early in the sampling schedule, correlating with aliasing artefacts in resulting spectra. By developing a convolutional screening approach to evaluate sampling schedules, these repeat sequences can be detected and characterized. Selecting schedules to avoid repeat sequences and using short periods of initial uniform sampling are effective at reducing these initial repeat sequences and enabling routine 25-33% 1D-NUS of challenging 2D-NMR experiments.

WEDNESDAY, APRIL 19, 2023 - *continued*

09:50-10:10 **SAND: Automated Time-Domain Modeling of NMR Spectra Applied to Metabolomics**

Presenting Author: Frank Delaglio

Yue Wu (Stanford University); Omid Sanati (University of Georgia); Mario Uchimiya (University of Georgia); Krish Krishnamurthy (Chempacker LLC); Art Edison (University of Georgia); Frank Delaglio (NIST IBBR)

NMR metabolomics offers great potential impact in drug discovery, diagnostics, and personalized medicine, but its exploitation requires detailed quantification of spectral features. Development of an automated, objective workflow for such quantification has been a long-standing challenge because of extensive spectral overlap and high signal complexity. To address this challenge, we introduce the software application SAND (Spectral Automated NMR Decomposition), for automated feature quantification in the time-domain. SAND follows upon the success of previous approaches to analyze spectra by time-domain modeling, adding a framework that provides automated quantification of entire spectra without the need for interactive region selection. We demonstrate SAND on metabolomics data including a urine spectral series spiked with differing amounts of a four-compound mixture.

WOB: BioSolution: Membrane Proteins (parallel session)
8:45 - 10:15, Chapel

08:45-09:10 **Structural and dynamic characterization of viral proteins: NS2B and domain III of glycoprotein E of Zika virus**

Presenting Author: Ana Paula Valente

Ana Paula Valente (Federal University of Rio de Janeiro)

We aim to explore fundamental issues associated with protein dynamics and macromolecular interactions in recognition processes using solution Nuclear Magnetic Resonance (NMR). We emphasize the study of NS2B and domain III of glycoprotein E of Zika virus. NS2B is a membrane protein responsible for regulating viral protease activity. We were able to elucidate its structure formed by four transmembrane helices and a hydrophilic portion that is compatible with the relaxation parameters and PRE data. The domain III of the glycoprotein E (DIII) is related to the binding of the virus to the cell receptor and neutralizing antibodies. DIII was studied free and in complex with glycosaminoglycan to mimic the interaction with the extracellular matrix.

09:10-09:30 **Bicelles Are an Effective Membrane Model for High-Resolution NMR Study of Curvature-Sensitive Molecules**

Presenting Author: Fang Tian

fang Tian (Penn State University College of Medicine); Yansheng Ye (Penn State University College of Medicine); Guifang Wang (Penn State University College of Medicine); Hong-Gang Wang (Penn State University College of Medicine)

Membrane curvature, a geometric measurement of the bending of the lipid bilayer, has been demonstrated to regulate enzymatic activity (e.g. ArfGAP1, Atg3, and Sar1) and direct the subcellular localization of some proteins (e.g. SpoVM and DivIVA). Our recent studies of human Atg3 (hAtg3) and VPS37A proteins demonstrated that, unlike micelles and nanodisc, bicelles are an effective membrane model for the structural study of curvature sensitive molecules, presumably because the loosely packed, dynamic planar surfaces of bicelles mimic a membrane with the type of packing defects that are required for interactions with these molecules.

09:30-09:50 **Ligands Tune the Local and Global Motions of Neurotensin Receptor 1 (NTS1): a Density-Functional Theory (DFT)-Guided Solution NMR Analysis**

Presenting Author: Joshua Ziarek

Joshua Ziarek (Indiana University)

Technical challenges have largely limited the application of NMR to the super-microsecond motional regimes of GPCRs. Focusing on a peptide-binding GPCR, the neurotensin receptor 1 (NTS1), we employed NMR and density functional theory to probe global sub-microsecond motions of 13Cε-methionine residues. Using this approach, known as methionine chemical shift-based global order parameters, we establish that the NTS1 solution ensemble includes substates with lifetimes on several discrete timescales. The longest-lived metastable states reflect those captured in agonist- and inverse agonist-bound crystal structures separated by large energy barriers. Individual methionine residues sense the rapid concerted motions superimposed within these long-lived states. The degree of these fast, global dynamics correlates with ligand pharmacology suggesting a role for conformational entropy in GPCR ligand discrimination.

WEDNESDAY, APRIL 19, 2023 - *continued*

09:50-10:15 **Conformational selection in GPCR activation and inhibition**

Presenting Author: Brian F Volkman

Brian Volkman (Medical College of Wisconsin); Shawn Jenjak (Medical College of Wisconsin); Roman R. Schlimgen (Medical College of Wisconsin); Andrew B. Kleist (Medical College of Wisconsin); Francis C. Peterson (Medical College of Wisconsin)

G protein–coupled receptors (GPCRs) recruit beta-arrestins to coordinate diverse cellular processes, but the structural dynamics driving this process are poorly understood. Atypical chemokine receptors (ACKRs) are intrinsically biased GPCRs that engage beta-arrestins but not G proteins, making them a model system to effector-specific signal transduction. 2D NMR experiments on native, 13C methionine–labeled ACKR3 revealed that beta-arrestin recruitment is associated with conformational exchange at key regions of the extracellular ligand-binding pocket and intracellular effector coupling region. Structure-function analysis of the nanobody-ACKR3 interface identified key contacts and reveal a novel mechanism for GPCR inactivation. Our data suggest that conformational selection guides -arrestin recruitment by tuning receptor dynamics at intracellular and extracellular regions.

WOC: *in vivo* Spectroscopy (parallel session)
8:45 - 10:15, Nautilus

08:45-09:10 **MR Spectroscopy Development of Metabolic Imaging Biomarkers in Gliomas**

Presenting Author: Changho Choi

Changho Choi (Vanderbilt University Medical Center)

Proton MR spectroscopy (MRS) of 2-hydroxyglutarate (2HG) and glycine in gliomas will be presented. Development of 2HG MRS and dissemination of the MRS protocol will be briefly discussed. In our study in 35 glioma patients, glycine level was positively correlated with cell proliferation rate and inversely correlated with expression of glycine decarboxylase enzymes. 2HG level did not correlate with cell proliferation rate. High level of glycine was significantly associated with short patient survival, irrespective of isocitrate dehydrogenase mutational status. Our data suggest that aggressive gliomas reprogram glycine-mediated one-carbon metabolism to meet the biosynthetic demands for rapid cell proliferation. MRS evaluation of 2HG and glycine may provide metabolic imaging biomarkers that are predictive of tumor progression and clinical outcome.

09:10-09:30 **Lactate Spectroscopy and Spectroscopic Imaging on a portable 46 mT Halbach MRI scanner**

Presenting Author: Itamar Ronen

Chloe Najac (C.J. Gorter Center for MRI, Department of Radiology, LUMC); Tom O'Reilly (C.J. Gorter Center for MRI, Department of Radiology, LUMC); Andrew Webb (C.J. Gorter Center for MRI, Department of Radiology, LUMC); Itamar Ronen (Clinical Imaging Sciences Centre, Brighton and Sussex Medical School, University of Sussex)

Low-field MRI systems (with B0<0.1T) for point-of-care applications are becoming increasingly widespread and could become a turning point for low-income countries and intensive care units. For magnetic resonance spectroscopy in vivo at low field, low SNR for biologically relevant molecules and lack of spectral separability pose significant challenges. Here we demonstrate the possibility of obtaining J-spectroscopic images of lactate solutions at B0=46mT using a Carr-Purcell-Meiboom-Gill (CPMG) sequence added with phase encoding gradients. Lactate spectra fit well with data acquired without spatial encoding and with density matrix simulations. Further work will focus on translating this methodology in vivo and accounting for the complexity of acquiring data in the human brain and other anatomies.

09:30-09:50 **Neural Network Reconstruction of Human Density-Weighted Concentric Ring Trajectory MRSI Data acquired at 3T**

Presenting Author: Nicholas Farley

Nicholas Farley (Purdue Univeristy); Uzay E. Emir (School of Health Sciences, Purdue University / Weldon School of Biomedical Engineering, Purdue University); Matt Rosen (MGH/Martinos Center); Neha Koonjoo (MGH / Martinos Center)

The previous decade saw significant improvements in computing hardware and software development tools which led to an increased interest in deep neural networks and their applications in mathematical problems such as data classification, feature extraction, noise reduction, and function emulation. Our group has attempted to train a deep neural network to learn the relationship between in-vivo Density-Weighted Concentric-Ring-Trajectory Spectroscopic k-space data and its corresponding Cartesian image-domain spectroscopic data. We show a direct comparison of outputs generated from our standard reconstruction pipeline and our neural network's inference. The metabolite peaks of NAA (~2ppm) and tCr (~3ppm) are noticeably well approximated.

WEDNESDAY, APRIL 19, 2023 - *continued*

09:50-10:15 **Magnetic Resonance Applications of Methyl Sulfone in vivo**

Presenting Author: Lana Kaiser

Ioannis Pappas (University of Southern California); Ben A. Inglis (University of California); Lana Kaiser (University of California)

Various applications of a common dietary supplement, methyl sulfone (MSM), are investigated in vivo using NMR and MRI methods. NMR properties of MSM in the healthy human brain and in the blood are examined regarding using MSM in vivo. Some of the applications include the usage as a chemical shift standard in vivo, a marker of the brain/gut axis in healthy aging and neurological diseases and the marker of the viability of blood/brain barrier. Preliminary results of using MSM to measure pH and temperature in the mammalian brain are summarized.

COFFEE BREAK with Exhibit Booths and Posters, Fireside Pavilion
10:15-10:45

WOD: Eclectica (parallel session)
10:45-12:35, Merrill Hall

10:45-11:10 **Zero- to ultralow-field NMR: some resent developments and applications**

Presenting Author: Dmitry Budker

Dmitry Budker (Helmholtz Institute, JGU Mainz and UC Berkeley)

In zero- to ultralow-field (ZULF) NMR, one does not need magnets in some or all of the three stages of an experiment: polarization, encoding, and detection. This unusual NMR modality has witnessed rapid development since the advent of compact and sensitive noninductive sensors, especially, atomic magnetometers that are now available commercially. In this talk we will discuss several recent ZULF NMR experiments carried out by our group and collaborators, demonstrating applications in areas as diverse as searches for beyond-the standard-model particles and interactions, monitoring chemical reaction dynamics within metal catalytic reactors, and detection of breaking down of membranes of biological cells as a result of chemotherapy. ZULF NMR may be combined with hyperpolarization and radioactive detection overcoming the sensitivity limitations.

11:10-11:30 **Optically Detected NMR of Photochemically Hyperpolarized Molecules**

Presenting Author: Danila Barskiy

Liubov Chuchkova (1. Institut fr Physik, Johannes Gutenberg Universitt-Mainz, 2. Helmholtz-Institut Mainz, GSI Helmholtzzentrum fr Schwerionenforschung); Roman Picazo-Frutos (1. Institut fr Physik, Johannes Gutenberg Universitt-Mainz, 2. Helmholtz-Institut Mainz, GSI Helmholtzzentrum fr Schwerionenforschung); James Eills (Institute for Bioengineering of Catalonia); Oleg Tretiak (1. Institut fr Physik, Johannes Gutenberg Universitt-Mainz, 2. Helmholtz-Institut Mainz, GSI Helmholtzzentrum fr Schwerionenforschung); Yinan Hu (State Key Laboratory of Brain and Cognitive Science, Institute of Biophysics, Chinese Academy of Sciences); Danila Barskiy (1. Institut fr Physik, Johannes Gutenberg Universitt-Mainz, 2. Helmholtz-Institut Mainz, GSI Helmholtzzentrum fr Schwerionenforschung); Sven Bodenstedt (ICFO-Institut de Cincies Fotniques, The Barcelona Institute of Science and Technology); Jacopo de Santis (ICFO-Institut de Cincies Fotniques, The Barcelona Institute of Science and Technology); Michael C. D. Tayler (ICFO-Institut de Cincies Fotniques, The Barcelona Institute of Science and Technology); Dmitry Budker (1. Institut fr Physik, Johannes Gutenberg Universitt-Mainz, 2. Helmholtz-Institut Mainz, GSI Helmholtzzentrum fr Schwerionenforschung, 3. Department of Physics, University of California); Kirill Sheberstov (Ecole Normale Superieure Paris)

Photochemically induced dynamic nuclear polarization (photo-CIDNP) enables nuclear spin ordering by irradiating a sample with light. An approach for measuring photo-CIDNP using fast-field-cycling NMR at nanotesla to microtesla fields is presented here for a model system. We demonstrate that photo-CIDNP can be optically detected for compounds with millimolar concentrations without isotopic enrichment. Spin hyperpolarization of protons higher than 0.1% was achieved by irradiating the sample with light at 20 mT. The proposed approach opens a new spectroscopic modality for spin-chemistry applications. Being insensitive to susceptibility-induced magnetic inhomogeneity, the method may be used to study relaxation rates at low fields and may help resolve open questions regarding the nature of avian magneto sensing.

WEDNESDAY, APRIL 19, 2023 - *continued*

11:30-11:50 **Enabling Operando 17O NMR of Lithium-Oxygen Batteries to Study Degradation**

Presenting Author: James H. J. Ellison

James Ellison (University of Cambridge); Clare P. Grey (University of Cambridge)

Lithium-Oxygen batteries (LOB) promise exceptional energy density, however, cells are very short lived, due to breakdown caused by reactive oxygen species. Operando 17O NMR being quantitative, non-invasive and real-time is a tantalising technique to study LOB.

We demonstrate that using enrichment, optimised CPMG/DFS and cell design, we can acquire spectra on the timescale of minutes. Gaussian processes are then used to fit the data and provide uncertainty estimates. We test to what extent degradation differs between electrochemical cycling and "rest" periods as well as observing changes in the amount of discharge/breakdown products with depth of charge and voltage applied, thus offering mechanistic insight to guide development of longer-lived cells. The methods generalise to operando studies of other similarly challenging nuclei.

11:50-12:10 **Iron Oxide Nanoparticle Quantification in Cryopreserved Rat Kidneys using Ultra Low Frequency Longitudinally-Detected Electron Paramagnetic Resonance (LOD-EPR)**

Presenting Author: Saurin Kantesaria

Saurin Kantesaria (University of Minnesota); XUEYAN TANG (University of Minnesota, Center for Magnetic Resonance Research); Steven Suddarth (University of Minnesota, Center for Magnetic Resonance Research); John Bischof (University of Minnesota, Department of Mechanical Engineering); Michael Garwood (University of Minnesota, Center for Magnetic Resonance Research)

Currently there is no low-cost method to nondestructively track IONPs in organs across a wide concentration range (0.05-100 mg Fe/mL). To address this, our lab has developed a low-cost, LOngitudinally Detected Electron Paramagnetic Resonance (LOD-EPR) system that can detect electron moments in IONPs. This work aims to evaluate LOD-EPR performance in terms of IONP quantification accuracy and effects of IONP behaviors such as particle aggregation on signal in solution and in biopsies of IONP-perfused rat kidneys. Linearity is demonstrated for LOD-EPR spectral peak amplitude vs concentration in 0.05-10 mg Fe/mL IONP samples. Aggregation decreases LOD-EPR signal intensity by ~50%. LOD-EPR signal is seen in IONP-perfused kidney biopsy compared to the baseline level signal in a fresh rat kidney biopsy.

12:10-12:35 **DNP Tensor Polarization Enhancement for Nuclear Physics Targets**

Presenting Author: Elena Long

Elena Long (University of New Hampshire)

Dynamic Nuclear Polarization targets have allowed for many spin observables to be measured in nuclear physics experiments. In spin-1 materials, the tensor polarization can also be enhanced and used to probe quark and nuclear structure. Tensor enhancement can be achieved by applying an additional semi-selective saturation RF in addition to microwave DNP enhancement. Such as system has been built at the University of New Hampshire for use in upcoming experiments at Jefferson Lab. Any overview of the process and target DNP system will be discussed.

WOE: BioSolids III (parallel session)
10:45-12:30, Chapel

10:45-11:10 **Magnetic-Alignment of Nanodiscs and NMR Applications**

Presenting Author: Ayyalusamy Ramamoorthy

Ayyalusamy Ramamoorthy (University of Michigan); Samuel McCalpin (University of Michigan); Bankala Krishnarjuna (University of Michigan); Thirupathi Ravula (University of Michigan)

A major focus of our research has been on the development of membrane mimetics (such as bicelles and nanodiscs) to enable the applications of solution and solid-state NMR experiments to study the dynamics structures of membrane-associated peptides and proteins. In this talk, the development of the nanodisc technology for NMR-based studies to probe the structural interactions between membrane-bound proteins such as cytochromes (~16-kDa b5, ~57-kDa P450, ~80-kDa P450-reductase) and to characterize membrane stabilized oligomeric amyloid intermediates will be presented. In addition, the use of magnetically-aligned nanodiscs to measure residual dipolar couplings (RDCs) and residual quadrupolar couplings (RQCs) from water-soluble biomolecules (such as proteins, RNA, and small molecules) will also be presented.

WEDNESDAY, APRIL 19, 2023 - *continued*

11:10-11:30 **2D DNP MAS NMR of Newborn Coral Shows that Glucose Diet Leads to Modulation of Polysaccharide and Protein Levels**

Presenting Author: Gil Goobes

Saja Nasser (Dpt of Chemistry, Bar-Ilan University); Maayan Neder (Dpt. of Marine Biology, Haifa University); Boran Uluca (Institute of Complex Systems, Juelich Research Center); Umit Akbey (Institute of Complex Systems, Juelich Research Center); Henrike Heise (Institute of Complex Systems, Juelich Research Center); Tali Mass (Dpt. of Marine Biology, Haifa University); Gil Goobes (Bar-Ilan University)

Hard coral homeostasis and skeletal calcification has been compromised by ocean acidification and temperature rise, disrupting cross-symbiont interactions between corals and guest photosynthetic alga. Newborn corals transform from swimming planula to polyps adhering to ocean bottom and producing protective exoskeleton. Knowledge of their skeletogenesis and tissue production are crucial to survivability under detrimental seawater conditions. Scleractinian corals feed on predation of a variety of small organisms and obtain nutrients from symbiont algae and resident gut bacteria. Direct impact of food source on either tissue or skeletal growth is unavailable.

We utilized Dynamic nuclear polarization to indicate changes in polysaccharide/protein profiles in planula and polyps by feeding with either 13C carbonate/glycine or 13C6-glucose/glycine and a metabolite associated with bacterial activity.

11:30-11:50 **Measuring Conformational Transitions in Cellular Prion Protein in Condensed Phases through 1D 13C NMR**

Presenting Author: Marcus Tuttle

Marcus Tuttle (Yale University); Yangyi Liu (Yale University); Haote Li (Yale University); Mikhail A. Kostylev (Yale School of Medicine); Daniel J. Walsh (Geisel School of Medicine at Dartmouth); Stephen M. Strittmatter (Yale School of Medicine); Surachai Supattapone (Geisel School of Medicine at Dartmouth); Victor Batista (Yale University); Kurt W. Zilm (Yale University)

Cellular prion protein (PrPC) has a structured C-terminal domain and an intrinsically disordered N-terminus. However, PrPC can also adopt additional phases, including a meta-stable conformation that undergoes maturation. Understanding these states is important to understanding PrPC's role in diseases such as Alzheimer's (AD) and prion diseases. To study these states, we developed a gradient descent-based method to resolve secondary structural distributions from a single 1D 13C NMR spectrum of a protein. We call this Secondary Structure Distribution by NMR (SSD-NMR). We validated SSD-NMR with over 1000 simulated spectra and from experimental data. We then use SSD-NMR to develop a model wherein PrPC LLPS is coupled to an equilibrium between canonical PrPC and a minor conformation with a more structured N-terminus.

11:50-12:10 **Structural Dynamics of Fungal Cell Walls and Remodeling by Osmotic Stress Elucidated by Solid-State NMR**

Presenting Author: Liyanage Devthilini Fernando

Liyanage Fernando (Michigan State University); Malitha Widanage (Louisiana State University); Frederic Mentink-Vigier (National High Magnetic Field Laboratory, Florida State University); Sungsool Wi (National High Magnetic Field Laboratory/FSU); Andrew S. Lipton (Environmental Molecular Sciences Laboratory); Nancy Washton (Enviromental Molecular Sciences Laboratory); Jean-Paul Latge (Unit des Aspergillus, Dpartement de Mycologie, Institut Pasteur); Tuo Wang (Michigan State University)

Here we present the use of multidimensional solid-state NMR and dynamic nuclear polarization (DNP) techniques for characterizing the polysaccharides and proteins in pathogenic fungi including Aspergillus, Candida, and Rhizopus species. The story, comprised of five recent studies, summarized how fungal cell wall is structured in mycelia and conidia, and how the structure changes in response to external stresses, such as antifungal drug and salinity, and internal factors, such as carbohydrate deficiency and mutation. These studies yield essential information about carbohydrate structures of the cell walls and their adaptations at atomic levels that can serve as potential targets for discovering novel antifungal compounds with broad spectrums and improved efficacy.

12:10-12:30 **Solid State NMR Characterization of Low Complexity Protein Sequence Assembly Mechanisms**

Presenting Author: Dylan T. Murray

Dylan Murray (University of California, Davis); Upasana Sridharan (University of California, Davis); Yuuki Wittmer (University of California, Davis); Blake Fonda (University of California, Davis); Khaled Jami (University of California, Davis); Estely Carranza (University of California, Davis); Kayla Osumi (University of California, Davis); Daniel Farb (University of California, Davis)

Proteins harboring low complexity amino acid sequences form organized and condensed assemblies functionally and pathologically in living cells. These proteins are challenging to study using solid state NMR due to their degenerate amino acid sequences. We present our approach using an existing computational assignment algorithm that has successfully yielded unambiguous results for four such proteins. We then illustrate the power of these results in characterizing the molecular mechanisms for the macroscopic assembly of these fascinating protein domains.

WEDNESDAY, APRIL 19, 2023 - *continued*

WOF: Small Molecules: Polarization, Methods (parallel session)
10:45-12:30, Nautilus

10:45-11:10 **Applying hyperpolarization to break sensitivity barriers of NMR for analysis of complex mixtures**

Presenting Author: Mathilde Hauge Lerche

Mathilde Lerche (Technical University of Denmark)

With hardware development, smart acquisition design and in tandem with other methodologies, the sensitivity drawback of NMR has been circumvented for numerous but specific applications. The potential of quantitative NMR is, however, far greater than currently exploited.

Hyperpolarization by dissolution dynamic nuclear polarization (dDNP) has recently been applied to enhance the resolution and sensitivity of NMR to detect compounds in complex mixtures. We have developed a stable isotope tracer-based hyperpolarized NMR method aiming to quantitatively measure metabolic flux with high sensitivity and high contrast. With this method metabolic pathways and networks can be mapped.

In the presentation we consider selected studies, discuss advantages and disadvantages of the hyperpolarization method in context of the studies and give perspectives to further developments.

11:10-11:30 **NMR and DNP Tools to Decipher Whole-Cell Catalysis: The Effect of Substrate Mixtures**

Presenting Author: Francesca Sannelli

Francesca Sannelli (Technical University of Denmark); Pernille Rose Jensen (Technical University of Denmark, DTU Heath Tech); Sebastian Meier (Technical University of Denmark, Chemistry)

NMR spectroscopy has been widely explored to study biochemical function in cells and biofluids. Non-natural modulation of intracellular chemistry by effectors often remains elusive. This response is relevant for a deep understanding of biochemistry, for engineering and for industrial bio-production with non-natural reactions using catalysts of close-to-zero cost, especially when engineering is not possible. NMR spectroscopy is adaptable and minimally invasive. Using NMR and dDNP-NMR, we found that bio-sourced substrate mixtures, can massively reroute the central metabolism of Baker's yeast toward formation of C-C bonds on furfural. Carbon from glucose sequesters to 80% adducts and only 20% ethanol. Studies on the influx of glucose from fermentation to minor pathways producing amino acid and industrial precursors are ongoing.

11:30-11:50 **NMR-Based Fragment Screening of Biomolecular Targets from the SARS-CoV-2 genome**

Presenting Author: Maria Alexandra Wirtz Martin

Maria Wirtz Martin (Goethe Universitt); Hannes Berg (Goethe Universitt); Sridhar Sreeramulu (Goethe Universitt); Christian Richter (Goethe Universitt); Verena Linhard (Goethe Universitt); Anna Niesteruk (Goethe Universitt); Harald Schwalbe (Goethe Universitt)

The emergence of the SARS-CoV-2 virus resulted in a worldwide pandemic that not only changed our everyday day life, but also has given birth to several research initiatives focusing on viral research and drug development. Within the COVID19-NMR, we undertook a massive research initiative involving world-wide NMR groups contributing towards the production, characterization and screening of viral proteins and RNA.

Fragment based screening by NMR aims to find compounds which act as starting points for the development of drugs. We have screened more than 20 RNA and 25 proteins, thus obtaining high quality hits. 311 binders across the 25 SCoV-2 proteins were identified and 69 binders were found that interact with different structured RNA elements in the SCoV-2 RNA genome.

WEDNESDAY, APRIL 19, 2023 - *continued*

11:50-12:10 **Parahydrogen Hyperpolarization as a Tool for Sensitivity Enhanced NMR Metabolomics**

Presenting Author: Indrek Reile

Kerti Ausmees (National Institute of Chemical Physics and Biophysics); Nele Reimets (National Institute of Chemical Physics and Biophysics); Sirje Vija (National Institute of Chemical Physics and Biophysics); Merle Uudsemaa (National Institute of Chemical Physics and Biophysics); Aleksander Trummal (National Institute of Chemical Physics and Biophysics); Indrek Reile (National Institute of Chemical Physics and Biophysics)

Parahydrogen hyperpolarization offers a relatively accessible way of increasing NMR signals by approximately three orders of magnitude over what is offered by the regular means of NMR sensitivity. Applied to chemical analysis of mixtures, this manifests in a substantial lowering of the limit of detection (LoD), allowing to adopt NMR in studies that may not be feasible otherwise.

We will show that parahydrogen hyperpolarization can be applied to analysis of human biofluids, allowing to access metabolic information from mid-nanomolar concentration analytes. We will show proof of concept applications for targeted metabolite analysis, demonstrate the feasibility of hyperpolarized spectral libraries and give examples of metabolite classes that we have analyzed by parahydrogen hyperpolarization (e.g., nicotinamide derivatives, nucleosides, nucleotides, oligopeptides).

12:10-12:30 **Applications of long-lived states of Methylene Protons in Achiral Molecules**

Presenting Author: Anna Sonnefeld

Anna Sonnefeld (Department of Chemistry, Ecole Normale Superieure); Aiky Razanahoera (Department of Chemistry, Ecole Normale Superieure); Philippe Pelupessy (Department of Chemistry, Ecole Normale Superieure); Geoffrey Bodenhausen (ENS); Kirill Sheberstov (Ecole Normale Superieure Paris)

Long-lived states have lifetimes that can be much longer than the longitudinal relaxation time. Here we show that proton long-lived states can be excited in common molecules containing neighboring methylene groups without the need for a chiral center, including neurotransmitters like γ-aminobutyric acid, acetylcholine and dopamine, and bioactive compounds like β-alanine, taurine and homotaurine. We show that long-lived states can be excited simultaneously in several molecules in a mixture and be used to enhance contrast in MRI experiments. This contrast can either be achieved by selective excitation and readout schemes that only address one component of a sample, or by exploiting differences in long-lived state lifetimes.

ASILOMAR LODGER LUNCH for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees may purchase a lunch ticket bundle or dinner ticket online by April 7.
12:45-14:00, Crocker Dinning Hall

POSTER SESSION with Exhibit Booths
14:00-15:45, Fireside Pavilion
See Poster Listings at end of document.

Tutorial and Award Session
16:00-18:00, Merrill Hall

16:00-16:35 **Tutorial - Hyperpolarization: An Overview of Principles, Methods, and Applications,** Boyd Goodson (*Southern Illinois University*)

16:35-17:10 **Tutorial - Low-Field NMR and MRI- Opportunities,** Mark Conradi (*ABQMR, Emeritus Washington University St. Louis*)

17:10-17:35 **Varian Young Investigator Awardee**

17:35-18:00 **Award Presentations (Students/Postdoc & Corp Vendor Contest)**

ASILOMAR LODGER DINNER for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees may purchase a lunch ticket bundle or dinner ticket online by April 7.
18:00 – 19:00, Crocker Dinning Hall

VENDOR HOSPITALITY SUITES
From 18:30

THURSDAY, APRIL 20, 2023

Early Morning Lecture Series (for Students & ALL who wish to learn!)
07:00-07:50, Merrill Hall

07:00-07:50 **Understanding NMR Spectroscopy** Part 4 of 4

Presenter: James Keeler

Would you like to deepen or brush up your understanding of NMR theory? Join us for a morning lecture series by **James Keeler** (University of Cambridge), author of *Understanding NMR Spectroscopy*. These lectures assume only a modest prior knowledge of NMR theory and will cover some key topics of wide interest to budding NMR spectroscopists. Topics will include: Energy levels, Hamiltonians and operators; Introducing and using product operators; Relaxation; Coherence selection by phase cycling and field gradients

ASILOMAR LODGER BREAKFAST for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees cannot purchase breakfast tickets, but you can purchase lunch and dinner tickets by April 7.
07:30-09:00, Crocker Dining Hall

ThOA: BioSolution: Structures and Methods (parallel session)
8:45 - 10:10, Merrill Hall

08:45-09:10 **A great peak picker, and what you can do with it: bioMolecule assignment, methylNOESYs, and Universal Saturation Transfer Analysis**

Presenting Author: Andrew J Baldwin

Andrew Baldwin (University of Oxford)

Virtually all NMR analysis requires peak picking (to get peak locations/shape/intensity). We present UnidecNMR, a deconvolution algorithm that (semi) automatically peak picks in 1-4D data, whose results match those of experienced users. This enables streamlined backbone assignment, and analysis of high molecular weight complexes via 4D methyl NOE data. Applying this to the saturation transfer experiment (uSTA) of complex 1D ligand spectra provides accurate ligand poses. Wiring this up to a Bloch-McConnell simulation, we also obtain reliable Kon/Koff and KD values. We use this to explore a range of ligand/protein interactions, including sugars binding COV19 Spike proteins. We've embedded this all in nice software so you can all test it out.

09:10-09:30 **Tackling a tripartite glycan conundrum: Flexibility/Sparse structural data/Signal resolution**

Presenting Author: Darón I. Freedberg

Daron Freedberg (CBER/FDA)

Despite the vast diversity of glycans, we face common, and often interconnected, challenges in their NMR structural studies: 1) discrimination of distinct conformations amongst a conformation-rich landscape, 2) limited structural data and 3) spectral overlap. We've addressed these issues by improving sensitivity and resolution, though not simultaneously. We will show that labile ¹H signals help alleviate two of these challenges and thus increase the repertoire of structural data. Ultimately, these help to discriminate unique conformations and refine structural models. I will also present methods to extract thermodynamic and kinetic data for conformational equilibria in glycans in the fast exchange. Finally, I will discuss our ongoing efforts to enhance the resolution for the structural studies of larger oligosaccharides.

09:30-09:50 **Analyzing AlphaFold Structures with NMR data**

Presenting Author: Joseph Sachleben

Isabelle Gagnon (University of Chicago); Tobin Sosnick (University of Chicago); Jeffery Ellena (University of Virginia); Urszula Derewenda (University of Virginia); Zygmunt Derewenda (University of Virginia); Eric Jonas (University of Chicago); Joseph Sachleben (University of Chicago)

The recent introduction of AlphaFold has fundamentally changed our ability to predict the structure of proteins from their primary sequence. We describe some straightforward NMR and computational methods to test these predicted structures. NOESY spectra provide a potential contact map between residues. TALOS torsion angles from backbone chemical shift constrain the predicted structure's secondary structure. We compare NMR data to the predicted structure of three proteins. We find that scores derived NMR data scale with the rmsd difference between predicted and determined structures. Further understanding of the NMR derived scores will be made by mining the data available on on-line data bases. Insights from this work will lead to new faster methods of NMR structural refinement and assignment.

THURSDAY, APRIL 20, 2023 - *continued*

09:50-10:10 **Ligand-capped Co(II) Multiplies the Value of the Double-Histidine Motif for PCS NMR Studies**

Presenting Author: Angela M. Gronenborn

Wenkai Zhu (University of Pittsburgh School of Medicine); Darian T. Yang (University of Pittsburgh School of Medicine); Angela Gronenborn (University of Pittsburgh School of Medicine)

In structural studies by NMR, pseudocontact shifts (PCSs) provide both angular and distance information. For proteins, incorporation of a di-histidine (diHis) motif, coordinated to Co2+ has emerged as an important tool to measure PCS. Here, we show that using different Co(II)-chelating ligands, such as NTA and IDA, resolves the isosurface ambiguity of Co2+-diHis and yields orthogonal PCS datasets with different Delta-chi tensors for the same diHis bearing protein. In addition, the use of capping ligands effectively eliminates undesired intermolecular interactions, mediated by metal binding, which can be detrimental for PCS studies. Devising and employing ligand-capping strategies afford versatile and powerful means to obtain multiple orthogonal PCS datasets, significantly extending the use of the diHis motif for structural studies by NMR.

ThOB: Hyperpolarization (parallel session)
8:45 - 10:10, Chapel

08:45-09:10 **Patches and Pockets of Weird Water -- Exploring New Frontiers with ODNP**

Presenting Author: John M Franck

Alec Beaton (Syracuse University); Alexandria Guinness (Syracuse University); Alexandria Guinness (Syracuse University); John Franck (Syracuse University)

Overhauser Effect Dynamic Nuclear Polarization (ODNP) utilizes resonant electron spins to enhance and isolate the properties of small pockets or patches of water in the hydration layer of large macromolecules. Here, it explores the dynamics of water trapped inside small pockets by surfactants, and water along the interface of a transmembrane protein and at the surface of a globular protein. These studies share a common theme that while ODNP easily analyzes viscous and phase heterogeneous samples containing large macromolecules or macromolecular complexes, it suffers from some difficulties by requiring low fields and operation in conjunction with a functioning EPR resonator. In overcoming some of these difficulties, we develop new methods for visualizing and resolving NMR signal.

09:10-09:30 **Steady-state Hyperpolarization of 1H in Liquids by Overhauser Dynamic Nuclear Polarization with 13C–1H Polarization Transfer**

Presenting Author: Yu Rao

Yu Rao (EPFL); Amrit Venkatesh (EPFL); Pinelopi Moutzouri (EPFL); Lyndon Emsley (EPFL)

Dynamic nuclear polarization (DNP) is a method that can significantly improve the sensitivity of NMR. The only effective DNP mechanism for in situ hyperpolarization in solution is Overhauser DNP, which is usually inefficient for 1H at high magnetic fields. Here we demonstrate the feasibility of exploiting the efficient Overhauser DNP on 13C to obtain significant steady-state 1H hyperpolarization in solution at high magnetic field. Using a 400 MHz gyrotron-equipped 3.2 mm MAS DNP system, we obtain 1H DNP enhancement factors of 48, 8, and 6 for chloroform, tetrachloroethane, and phenylacetylene, respectively, at room temperature.

09:30-09:50 **Structural Description of CaCO3 Prenucleation Clusters through 13C MAS-DNP NMR**

Presenting Author: Thierry Azaïs

Thierry Azais (Sorbonne Universite); Tristan Georges (Sorbonne Universite); Vinavadini Ramnarain (IPCMS); Christel GERVAIS (LCMCP - Sorbonne Universite); Clment Sanchez (Collge de France); Ovidiu Ersen (IPCMS)

Calcium carbonate (CaCO3) is one of the most significant biominerals in Nature found in the skeletons of sea urchins, cuticles of crustaceans, mollusks shells or corals. It was recently shown that CaCO3 crystallization is occurring through a non-classical nucleation pathway for which various intermediate phases are involved. In this communication, we show that 13C MAS-DNP NMR allows the comprehension of the initial step of CaCO3 nucleation including the structural atomic description of CaCO3 prenucleation clusters. This method combines two advantages (i) the sensitivity enhancement induced by DNP, particularly useful for physiological concentration (1-4 mM), but also (ii) the low temperature that is quenching the nucleation process and allow the stabilization of such transient species.

THURSDAY, APRIL 20, 2023 - *continued*

09:50-10:10 **Study of Gadolinium Effects in the Hyperpolarization of [15N3]Metronidazole: an FDA-approved Antibiotic and Potential Hypoxia Probe**

Presenting Author: David O. Guarin Bedoya

David Guarin Bedoya (Athinoula A. Martinos Center for Biomedical Imaging, Department of Radiology, Massachusetts General Hospital); Sameer M. Joshi (Department of Chemistry, Integrative Biosciences (Ibio), Karmanos Cancer Institute (KCI), Wayne State University,); Anna Samoilenko (Department of Chemistry, Integrative Biosciences (Ibio), Karmanos Cancer Institute (KCI), Wayne State University); Mohammad S. H. Kabir (Department of Chemistry, Integrative Biosciences (Ibio), Karmanos Cancer Institute (KCI), Wayne State University); Erin E. Hardy (Department of Radiology, Athinoula A. Martinos Center for Biomedical Imaging, Massachusetts General Hospital, 149 13th St.); Atsushi M. Takahashi (Department of Brain and Cognitive Sciences, McGovern Institute for Brain Research, Massachusetts Institute of Technology); Jan H. Ardnkjaer-Larsen (Department of Health Technology, Technical University of Denmark, 348, rsteds Pl.,); Eduard Y. Chekmenev (Department of Chemistry, Integrative Biosciences (Ibio), Karmanos Cancer Institute (KCI), Wayne State University); Yi-Fen Yen (Athinoula A. Martinos Center for Biomedical Imaging, Department of Radiology, Massachusetts General Hospital)

In this work, we hyperpolarized [15N3]metronidazole(MNZ) with dynamic nuclear polarization(DNP) technique. Metronidazole is an FDA-approved antibiotic that can be potentially employed as a hypoxia-sensing probe. A good polarization (~6%) was achieved with very short polarization build-up time constants (~12min) and,T1 and T2 of 343 s and 20 s in liquid-state respectively. We used Electron Paramagnetic Resonance(EPR) spectroscopy to show that a sample of [15N3]MNZ + trityl AH111501 had narrower EPR linewidth and larger magnitude than AH111501 alone, indicating an efficient polarization transfer from the radical electrons to 15N and supporting our observations of fast DNP buildup. We also demonstrated that the addition of a gadolinium-based compound to the [15N3]MNZ+AH111501 sample broadened the EPR spectrum and prolonged DNP buildup as observed.

ThOC: Rethinking What We Know in MRI (parallel session)
8:45 - 10:10, Nautilus

08:45-09:10 **Hemodynamic brain mapping with high-field (14T) preclinical fMRI methods**

Presenting Author: Xin Yu

Xin Yu (MGH)

"Functional" MRI is developed to map neurovascular coupling-based hemodynamic changes, i.e. the CBV, CBF, and BOLD signals, as indirect measures of neuronal activity. Despite existing spatial specificity functional mapping studies, one intriguing question is "what can we detect when the spatial resolution is improved from the millimeter to the tens-of-micron scale?" Here, I will present two sets of high-resolution fMRI methods: line-scanning fMRI and single-vessel fMRI, using the 14T MRI scanner. The line-scanning fMRI allows laminar hemodynamic mapping with 50-micron resolution and 5-to-50ms sampling rates. The single-vessel fMRI enables the detection of arteriole and venule (20-70 micron)-specific hemodynamic responses across different brain regions in animals. Both methods enable the circuit-specific or vessel-specific hemodynamic mapping of awake transgenic mouse models.

09:10-09:30 **Assess Gas Flow field of the Lung using High Spatiotemporal Resolution Dynamic Hyperpolarized 129Xe MRI**

Presenting Author: Haidong Li

Hongchuang Li; Ming Zhang; Xiaoling Liu; Xiuchao Zhao, Yeqing Han; Chaohui Ye; Xin Zhou (National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences, Wuhan, China)

Noninvasively imaging dynamic ventilation with high spatiotemporal resolution is of great demand for diagnosing lung diseases that related to obstructive ventilation. Unfortunately, limited by the short breathing cycle, it is difficult to obtain high temporal resolution and quantitatively analyze the airflow distribution. In this study, we propose a method for obtaining dynamic ventilation images with super-spatiotemporal-resolution via hyperpolarized 129Xe MRI, and obtain the flow field of hyperpolarized 129Xe gas in the lung by drawing lessons from optical flow methods. Our preliminary results demonstrated the feasibility of the optical flow methods for evaluating dynamic ventilation function regionally in vivo, which would be helpful for assessing the pathological changes of the lung caused by the diseases that related to dynamic ventilation abnormality.

THURSDAY, APRIL 20, 2023 - *continued*

09:30-09:50 **Development of a Compact NMR System to Measure pO2 in a Tissue-Engineered Graft**

Presenting Author: Efrain Torres

Efrain Torres (University of Minnesota); Saurin Kantesaria (University of Minnesota); Paul Wang (University of Minnesota); Parker Jenkins (University of Minnesota); Leah Steyn (The University of Arizona); Lance DelaBarre (University of Minnesota); Taylor Froelich (University of Minnesota); Daniel Pizetta (University of Sao Paulo); Dimitrios Sakellariou (KU Leuven); Alberto Tannus (University of Sao Paulo); Klearchos Papas (The University of Arizona); Michael Garwood (University of Minnesota)

A tissue-engineered graft (TEG) containing islet cells could serve as a bioartificial pancreas when implanted in the forearm of diabetic patients. The bioartificial pancreas requires supplemental oxygen delivery to ensure oxygen remains within physiological levels1. To monitor its oxygen levels, TEGs contain perfluorocarbons with oxygen-sensitive R1 values2. Here we present a tabletop oxygen scanner based on 19F NMR relaxometry. The system will be used in research and upcoming clinical trials evaluating a potential cell-based functional cure for type I diabetes.

09:50-10:10 **High Resolution MRI with Low Amplitude Gradient**

Presenting Author: Dan Xiao

Mark Armstrong (University of Windsor); Dan Xiao (University of Windsor)

The Pi Echo Planar Imaging (PEPI) sequence employs multiple refocusing RF pulses and unbalanced spatial encoding gradients. The phase accumulates throughout the entire echo train, so that the gradient duty cycle can be drastically reduced compared to fast spin echo (FSE). A shorter echo spacing may also be achieved. PEPI requires near ideal 180° refocusing pulses to eliminate the coherence pathway artifacts, which has limited its application to 3D imaging of small samples confined to the homogeneous region of the RF coil. Sufficient quality 2D PEPI could not be obtained due to the imperfect slice profile. In this work, an optimized phase cycling scheme is proposed to minimize coherence pathway artifacts with non-ideal refocusing pulses and enable 2D PEPI imaging.

COFFEE BREAK with Exhibit Booths and Posters, Fireside Pavilion
10:20-10:45

ThOD: Methodology and Applications of Inorganic Materials (parallel session)
10:45-12:35, Merrill Hall

10:45-11:10 **1H CSA: Friend or Foe?**

Presenting Author: Frederic A. Perras

Scott A. Southern (Ames National Laboratory); Takeshi Kobayashi (Ames National Laboratory); Alexander Paterson (University of Wisconsin-Madison); Yusuke Nishiyama (JEOL Ltd.); Frederic Perras (Ames National Laboratory)

Despite the high sensitivity, and recent resurgence, of 1H solid-state NMR, measurements of 1H chemical shift anisotropy (CSA) have remained rather niche. In many instances, we would even consider it a nuisance that leads to decoherence and t1 noise in 1H dipolar recoupling. This presentation will cover the development of highly stable dipolar recoupling methods that decouple the 1H CSA in addition to new 1H CSA recoupling schemes that enable the measurement of tensor skew, and small anisotropies. Lastly, the utility and limitations of 1H CSA for the measurement of dynamic information in low-sensitivity samples, such as heterogeneous catalysts, will be discussed.

11:10-11:30 **Solid-state NMR Characterizations of the Reorientational Dynamics of A-site Cations in 2D Organic-Inorganic Hybrid Perovskite**

Presenting Author: Tsyr-Yan Dharma Yu

Cheng-Chieh Lin (NTU-MST, National Taiwan University); Shing-Jong Huang (Instrumentation Center, National Taiwan University); Pei-Hao Wu (Institute of Atomic and Molecular Sciences, Academia Sinica); Vladimir M. Gelev (Department of Chemistry and Pharmacy, Sofia University); Chun-Wei Chen (Department of Materials Science and Engineering, National Taiwan University); Tsyr-Yan Yu (Institute of Atomic and Molecular Sciences, Academia Sinica)

Organic–inorganic hybrid perovskites (OIHPs) have attracted a significant amount of attention for photovoltaic applications since their power conversion efficiency has reached over 25%. Limited methods are available for investigating the reorientational dynamics of A-site cations in 2D OIHPs, which play a pivotal role in determining their physical properties. We characterized the dynamics of A-site cations using isotope labelling combined with ssNMR methods. While 2H NMR analysis reveals the existence of multiple modes of reorientational dynamics of methylammonium, REDOR NMR of 2D OIHPs incorporating (13C,15N)- methylammonium reflects the averaged dipolar coupling between the two nuclei undergoing different modes of motions. The interplay between the rigidity of the organic spacers and the A-site cations dynamics of 2D OIHPs is clearly revealed.

THURSDAY, APRIL 20, 2023 - *continued*

11:30-11:50 **Rapid dynamic nuclear polarization with conductive polymers**

Presenting Author: Quentin Stern

Quentin Stern (UCBL); Guillaume Verhaeghe (UCBL); Tho El-Dara (UCBL); Charlotte Bocquelet (UCBL); Sami Jannin (UCBL)

Dissolution dynamic nuclear polarization (dDNP) uses the high polarization of electron spins at low temperatures to polarize nuclear spins to near-unity levels on a broad variety of compounds. After dissolving the sample, this hyperpolarization translates into sensitivity gains for liquid-state NMR and MRI of up to five orders of magnitude. Here, we show that DNP is feasible on polyaniline polymers (PANI) at 1.6 K and 7 T and find a surprising variety of DNP mechanisms as a function of radical concentration. DNP on PANI opens the perspective of efficient DNP at moderate temperatures and hence, without the need for liquid helium since electrons in chiral PANI can be hyperpolarized by chirality-induced spin selectivity.

11:50-12:10 **Cross Polarization from Dipolar-Order under Magic Angle Spinning: The ADRF-CPMAS NMR Experiment**

Presenting Author: Tamar Wolf

Tamar Wolf (Weizmann Institute of Science); Lucio Frydman (Weizmann Institute of Science)

Techniques for enhancing low-gamma X-spin signals are crucial in solid-state NMR. The leading method to sensitize unreceptive X nuclei is Hartmann-Hahn cross polarization (HH-CP), often executed under MAS. Herein, we explore the possibility of utilizing 1H dipolar order created via adiabatic demagnetization in the rotating frame (ADRF), to enhance the X-spins under MAS. Somewhat unexpectedly, we find that an efficient polarization transfer via ADRF-CPMAS can be possible, exceeding in some instances that of an optimized HH-CPMAS. The experiment requires low-powers on both the 1H and the X channels, and displays unusual zero- and double-quantum matching conditions. These are analytically derived and numerically simulated, in predictions that compare well with experimental 13C and 15N results collected at different spinning speeds.

12:10-12:35 **Nuclear Spins as Probes of Electronic States in Semiconductors and the "Spin Bath" - What Can We Learn from Hyperpolarization via Optical Pumping**

Presenting Author: Sophia Hayes

Weijian Chen (Washington University); Michael West (Washington University)

Optically-pumped NMR in CdTe and GaAs is still yielding insights into both the electronic states in the semiconductors as well as the behavior of the "spin bath". A grand challenge in quantum technologies is the preservation of spin coherence lifetimes. Spin systems that coherently couple to light offer key capabilities for quantum technologies. Here we report on long nuclear spin coherence lifetimes of ^{113}Cd in CdTe that have been polarized through coupling to optically-oriented electrons.

ThOE: Techniques for Small Molecules (parallel session)
10:45-12:35, Chapel

10:45-11:10 **Novel and Robust Conformational Analysis to Advance 3D Structure Characterization of Cyclic Peptides**

Presenting Author: Qi Gao

Qi Gao (Merck); Xiao E. Wang (Merck); Ajay N. Jain (BioPharmics LLC); Edward N. Sherer (Merck); Mikhail Reibarkh (Merck)

The interest in macrocyclic peptides as new scaffolds in the development of novel drugs has significantly increased owing to their potential to interact with novel and challenging biological targets. Facile and precise elucidation of the 3D conformation of such molecules can provide insight into structure-activity relationships, which in turn illuminates molecular design toward improving pharmacological performance. We will present a newly developed approach featuring rapid determination of high-resolution 3D conformational ensembles of cyclic peptides and macrocycles in solution using a small number of NMR restraints using an advanced conformational sampling algorithm. The methodology developed can be applied to many therapeutic peptides and has the potential to contribute to developing novel medicines by enabling rapid access to high-resolution solution conformations.

THURSDAY, APRIL 20, 2023 - *continued*

11:10-11:30 **Operando Metabolomics of Healthy and Cholestatic Liver Tissue Slices By Microfluidic NMR**

Presenting Author: Marcel Utz

Bishnubrata Patra (University of Southampton); Manvendra Sharma (University of Southampton); Ruby Karsten (University of Groningen); Sabeth Verpoorte (University of Groningen); Jan G. Korvink (Karlsruhe Institute of Technology); Marcel Utz (University of Southampton)

A microfluidic platform is described that allows in-situ observation of metabolic processes in live murine liver tissue slices. The system is based on a transmission-line NMR microprobe, which is designed to accommodate a microfluidic chip that holds the tissue slice, and ensures nutrient and oxygen supply, as well as gas exchange and temperature stability.The system is capable of quantifying metabolic production/consumption rates of more than 20 different metabolites from a single tissue slice, with a time resolution of a few minutes.

11:30-11:50 **Integrated Approach of J-resolved STOCSY and INADEQUATE in 13C NMR Metabolomics**

Presenting Author: Mario Uchimiya

Mario Uchimiya (University of Georgia); Malin Olofsson (University of Georgia); McKenzie A. Powers (University of Georgia); Brian M. Hopkinson (University of Georgia); Mary Ann Moran (University of Georgia); Arthur S. Edison (University of Georgia)

Robust annotation of metabolites is a critical task in metabolomics. 13C-experiment INADEQUATE is an ultimate experiment that provides definitive structure based on carbon networks. Despite its utility, it is not always practical to collect INADEQUATE on every sample in a large study because of its relatively long experiment time. Here, we propose an alternative that integrates 13C homonuclear JRES, STOCSY, and INADEQUATE information. We tested this approach using the 13C-labeled endometabolome of a model marine diatom. This approach extracted both known and unknown diatom metabolites with structural information. The ability of this scheme was seen even in sugar regions, which are usually challenging due to severe peak overlap. This approach can maintain the quality of information but saves experiment time.

11:50-12:10 **Ultrafast diffusion NMR: an emerging tool for the analysis of mixtures**

Presenting Author: Rituraj Mishra

Rituraj Mishra (University of Nantes); Jonathan Yong (University of Oxford); Achille Marchand (University of Nantes); Corentin Jacquemmoz (Direction gnrale de l'Armement); Mohammadali Foroozandeh (University of Oxford); Jean-Nicolas Dumez (University of Nantes)

SPatially ENcoded Diffusion Ordered Spectroscopy (SPEN-DOSY) has emerged as a new time-efficient tool for the analysis of mixtures of small molecules in solution. Time efficiency is achieved using the concept of spatial parallelization of the effective gradient area and the data is processed by least-squares optimization to extract diffusion coefficients. The overlapping peaks, however cannot be separated and identified via such processing. We have implemented multivariate processing methods, DECRA, SCORE, OUTSCORE, and a recent univariate processing method, Matrix Pencil Method (MPM) for the separation of such overlap. However, as the number of components increases, it becomes difficult to separate them even with these methods. This limitation is addressed via using the PSYCHE sequence to record SPEN-DOSY NMR data.

THURSDAY, APRIL 20, 2023 - *continued*

ThOF: Instrumentation II (parallel session)
10:45-12:30, Nautilus

10:45-11:10 **Frequency Modulation and DNP**

Presenting Author: Daphna Shimon

Daphna Shimon (The Hebrew University of Jerusalem)

In a standard dynamic nuclear polarization (DNP) experiment, we irradiate at a constant microwave (MW) frequency and observe the DNP enhancement of the nuclear signal. Recently, several groups have begun introducing frequency modulation (FM) of the MW irradiation. With FM, it is possible to affect more electron spins during the DNP experiment, often leading to an increase in the DNP enhancement. When several DNP mechanisms are active in the same sample, FM can also cause a change in the relative contribution of each mechanism. In this work, I will discuss performing FM and how it affects the various DNP mechanisms.

11:10-11:30 **Fabrication and Testing of Solenoids Optimized from System-Defined Constraints**

Presenting Author: Jessica I. Kelz

Jessica Kelz (UC Irvine); Jose L. Uribe (UC Irvine); Robert G. Marosi (UC Irvine); Filippo Capolino (UC Irvine); Rachel W. Martin (UC Irvine)

Solenoids are a common transceiver in NMR probes due to robust performance and relative ease of utilization, however published optimizations are limited. We developed a generalized approach that readily enables design and fabrication of solenoids optimized for homogeneity based on instrument-specific constraints using a Biot-Savart approximation. 3D-printed coil templates will be used to fabricate generated 3.2mm designs for a MAS probe including constant-pitch to maximize B1 and variable-pitch to maximize axial homogeneity. Field profiles will be benchtop tested using a high-resolution and automated ball-shift apparatus to assess any limitations prior to further experimental validation. This process is accessible to all instrumentation skill levels, time efficient, can improve performance, and has the potential to benefit more complicated designs in the future.

11:30-11:50 **A Low-Field Permanent Magnet Magnetic Resonance Instrument Designed for Multimodal Imaging: Application in the GAMMA-MRI Project**

Presenting Author: Dimitrios Sakellariou

Rodrigo de Oliveira-Silva (KU Leuven); Tomas Rodriguez (Inspiralia); Renaud Jolivet (Maastrich University); Luis Fraille (Universidad Complutense de Madrid); Magdalena Kowalska (CERN); Jean Noel Hyacinthe@hesge.ch (University of Applied Sciences of Western Switzerland); Julien Rivoire (RS2D); Stavroula Pallada (7HES-SO University of Applied Sciences of Western Switzerland); Dimitrios Sakellariou (KU Leuven)

Low-field magnetic resonance is witnessing renewed interest in the light of permanent-magnet based assemblies that offer transportability, low-cost in acquisition/maintenance, improved sustainability, as well as additional options for innovative customized design. This becomes appealing when MRI is combined with other imaging modalities, and/or even other detection/hyperpolarization methodologies. The GAMMA-MRI project is exploring the possibility to apply MR techniques to spatially encode the photons of hyperpolarized xenon isotopes emission and detecting using gamma detectors surrounding the imaged object. This mode of detection promises improving the limits of detection while maintaining the advantages of high-field MRI. A low-field MRI instrument will be presented which has been custom-designed and build complying with multiple constrains without impacting the quality of the MRI imaging.

11:50-12:10 **NMRduino: a modular, open-source platform for dc and low-field magnetic resonance**

Presenting Author: Michael Tayler

Sven Bodenstedt (ICFO - The Institute of Photonic Sciences); Michael Tayler (ICFO - The Institute of Photonic Sciences)

The "NMRduino" is a single-board magnetic resonance spectrometer based on Arduino that we have developed over recent years to study hyperpolarized NMR systems, fast-field-cycling NMR relaxation, high-resolution spectroscopy, and coherent control at low magnetic fields, as well as teach basic principles of magnetic resonance to student beginners. Having undergone several design iterations and extensive testing, it is ready for community release. In this presentation, we would like to discuss NMRduino's capabilities and show how you can obtain and use it. Main features and applications in latest research will be demonstrated.

THURSDAY, APRIL 20, 2023 - *continued*

12:10-12:30 **Simplifying in-situ photochemical analysis with NMRtorch**

Presenting Author: Wendy Nason-Palmer

Jack E. Bramham (University of Manchester); Wendy Nason-Palmer (Oxford Instruments Inc.); Robin J. Blagg (Oxford Instruments); James Sagar (Oxford Instruments); Alexander P. Golovanov (University of Manchester)

Much of chemistry is photo sensitive, whether that is biological reactions, catalysts, photo switches or degradation. NMR is an excellent tool for characterising the photosensitivity of chemicals or materials due to inherent richness of NMR information and the lack of reliance on optical detection. Here we present a new approach for In-situ photo NMR, NMRtorch. Thich enables convenient and portable in-situ sample illumination without optical fibres or probehead modifications, and can be easily moved between NMR systems, whether benchtop or high field. We will introduce the principles of this approach and demonstrate its performance in several typical photo-NMR applications including photo degradation, photoisomerization and photochemically induced dynamic nuclear polarisation (pCIDNP).

ASILOMAR LODGER LUNCH for attendees lodging at Asilomar. Asilomar lodgers will receive meal tickets at check-in. Off-site attendees may purchase a lunch ticket bundle or dinner ticket online by April 7.
12:45-14:00, Crocker Dinning Hall

POSTER SESSION
14:00-15:45
See Poster Listings at end of document.

ThOG: BioSolids IV (parallel session)
16:00 - 17:45, Merrill Hall

16:00-16:25 **High sensitivity NMR for structural determination of neurodegenerative disease-associated proteins inside cells**

Presenting Author: Kendra K Frederick

Kendra Frederick (UTSouthwestern)

The misfolded proteins associated with neurodegenerative disease can adopt a variety of different conformations, some of which are toxic. Because these proteins have identical amino acid sequences, the cellular environment clearly influences the final state, yet most structural studies do not include the cellular context and, perhaps because we are not studying the correct conformation, not a single therapeutic strategy for these diseases addresses the underlying protein misfolding pathology. Using new sensitivity-enhancement technology for solid state NMR spectroscopy, Dynamic Nuclear Polarization, we study protein structure in native environments - inside living cells - to reveal how both healthy and disease-relevant cellular environments influence protein structure.

16:25-16:45 **Structural insights into the Biofilm Forming Functional Amyloids**

Presenting Author: Umit Akbey

Umit Akbey (Structural Biology, University of Pittsburgh)

Aggregated proteins in the form of amyloid fibrils play a key role/function (functional amyloids) in maintaining the structural integrity of bacterial biofilms. Such functional amyloids strengthen biofilms and are a major threat to human health, since the (chronic) infections they cause are difficult to treat due to the biofilm structural integrity and insufficient penetration of drugs, thus promoting antibiotic resistance (antimicrobial resistance, AMR).

Here, I will present our recent work on NMR spectroscopy based structural characterization of several functional amyloids. Moreover, results from other strutural techniques and biophysical characterization will be presented.

16:45-17:05 **Intrinsic protein disorder in the solid state: a combined solid-state NMR and EPR approach**

Presenting Author: Ansgar Siemer

Sayuri Pacheco (USC); Silvia Cervantes (USC); Dhanya Reselammal (USC); Ansgar Siemer (USC)

When studying intrinsically disorders protein domains (IDDs), a strength of NMR spectroscopy is to provide local structural information via chemical shifts and dynamics via relaxation rates and residual dipolar couplings. A strength of (DEER) EPR, in this context, is to provide distance distributions with unambiguous assignments, making it very complementary to NMR spectroscopy. Here, we use both NMR and EPR in combination with MD simulations to define the conformational ensemble of IDDs that are often found on the surface of cross-β fibrils important in neurodegenerative diseases. In addition, we use a combination of solid-state and solution NMR techniques under MAS to determine the binding site of the co-chaperone DNAJB1 to these IDDs.

THURSDAY, APRIL 20, 2023 - *continued*

17:05-17:25 **Atomic-Resolution Magic-angle spinning NMR Structure of the Protein Encoded by Gene V of fd phage in Complex with its full-length Viral ssDNA**

Presenting Author: Amir Goldbourt

Amir Goldbourt (Tel Aviv University)

Single stranded filamentous bacteriophage viruses undergo an intermediate step where thousands of homodimers of a non-structural protein, gVp, bind newly synthesized strands of DNA, preventing further DNA replication and signaling assembly of new virions at the membrane. Past studies have only been able to model the ssDNA-bound conformation using X-ray and solution NMR structures of isolated dimers. We report here an atomic-resolution magic-angle spinning solid-state NMR structure of a monomer of gVp within the context of an 8233-nucleotide-long ssDNA in the nucleoprotein complex. The model presents significant conformational changes, having a backbone r.m.s.d. of 6.4Å with respect to the free form. We show how these modifications facilitate ssDNA binding mechanism and promote the reported cooperative binding generating the cellular assembly.

17:25-17:45 **Coherent DNP with Chirped Pulses**

Presenting Author: Yifan Quan

Yifan Quan (MIT); Manoj Subramanya (National High Magnetic Field Laboratory); Yifu Ouyang (MIT); Michael Mardini (Massachusetts Institute of Technology); Thierry Dubroca (National High Magnetic Field Laboratory); Stephen Hill (National High Magnetic Field Laboratory); Robert Griffin (Massachusetts Institute of Technology)

We present a study of coherent dynamic nuclear polarization (DNP) using frequency swept pulses at 94 GHz (W-band). Using chirped pulses, the polarization transfer efficiency can be optimized and an enhancement ε ~ 496 was observed using 10 mM trityl-OX063 as the polarizing agent in a standard d8-glycerol:D2O:H2O: 6:3:1 glassing matrix at 70K. The frequency swept pulses enhance the nuclear magnetic resonance (NMR) signal, and also reduce the recycle delay, accelerating the NMR signal acquisition.

ThOH: Quantum Calculations of NMR Parameters (parallel session)
16:00 - 17:50, Chapel

16:00-16:25 **The Importance of Nuclear Quantum Effects (Nuclear Delocalization) for Hydrogen Bonding and for Predictions of NMR Parameters**

Presenting Author: Martin Dracinsky

Martin Dracinsky (Institute of Organic Chemistry and Biochemistry)

Hydrogen atom is intrinsically quantum mechanical and nuclear quantum effects (NQEs), such as nuclear delocalization and tunneling are important for its properties. NMR spectroscopy provides a tool for the investigation of NQEs. Recent progress in combining experimental NMR with path-integral molecular dynamics (PIMD) simulations that include NQEs will be discussed. We used this combination of experiment and theory to investigate resonance stabilization of hydrogen bonds and for accurate predictions of isotope shifts. We have also investigated salt-to-cocrystal transformations of multicomponent pharmaceutical solids. A combination of solid-state NMR spectroscopy with DFT-PIMD simulations provides evidence of temperature-induced hydrogen-atom shift in cocrystals with short hydrogen bonds. The hydrogen atom can be significantly delocalized between the acid and the base, forming a hydrogen-bond continuum.

16:25-16:45 **A New Route to Chemical Shieldings and their Intrepretation from First Principles Computations**

Presenting Author: Josef W. Zwanziger

Josef Zwanziger (Dalhousie University)

We have developed a new formalism for calculating chemical shielding in solids and implemented it in the Abinit code. This new approach lets us determine the different contributions of the electronic bands to the shielding tensor, opening the way to detailed interpretation and chemical insight based on the individual orbital contributions. Our approach is based on a perturbative expansion of the total energy as a function of the magnetic field, making use of magnetic translation symmetry. This approach yields a band-by-band decomposition of the shielding and hence direct interpretation in terms of orbitals. We will discuss details of our implementation and examples and comparisons with other approaches.

THURSDAY, APRIL 20, 2023 - *continued*

16:45-17:05 **Relativistic DFT Calculations of NMR Parameters for the Platinum Group Elements**

Presenting Author: Sean Holmes

Sean Holmes (Florida State University); Jasmin Schnzart (Florida State University); Adam Philips (University at Buffalo); Jochen Autschbach (University at Buffalo); Robert Schurko (Florida State University)

The platinum group elements (PGEs), which include Rh, Ru, Pd, Os, Ir, and Pt, are widely used in catalysts, optical devices, sensors, alloys, and many other advanced materials, due to their unique covalent donation bonding. The combination of solid-state NMR (SSNMR) spectroscopy and density functional theory (DFT) calculations affords a unique opportunity to gain insights into this bonding. DFT calculations are invaluable for relating chemical shift (CS) and electric field gradient (EFG) tensors to molecular-level structure and bonding. Herein, we discuss the development and application of relativistic computational methods for calculating the NMR parameters for the PGEs, as well as CS tensors for light ligand atoms bonded to PGEs, and their interpretation in terms of electronic structure and bonding.

17:05-17:25 **High Precision Structures of Cellulose Polymorphs Obtained with an NMR Crystallography Approach**

Presenting Author: Darren Brouwer

Darren Brouwer (Redeemer University)

The detailed structural characterization of cellulose has presented numerous challenges due to its fibrous nature and multiplicity of crystalline forms and there remain outstanding questions, particularly concerning the hydrogen-bonding networks within and between cellulose chains. Fibre neutron and X-ray diffraction experiments have provided structures for the various forms of cellulose, however there are intrinsic limitations to the precision that can be achieved with fibre diffraction Here, it is shown that an "NMR crystallography" approach, in which SSNMR results and DFT calculations are combined, provides high precision structures of four of the polymorphs of cellulose.

17:25-17:50 **Speeding up CASE-3D with machine learning prediction of scalar couplings and chemical shielding tensors**

Presenting Author: Armando Navarro-Vázquez

Armando Navarro-Vazquez (Universidade Federal de Pernambuco); Alejandro Tanguma (Departamento de Qumica, Cinvestav); Higo de Araujo Oliveira (Departamento de Qumica Fundamental, Universidade Federal de Peranmbuco); Wildson Jose de Almeida Ramos (Departamento de Qumica Fundamental, Universidade Federal de Pernambuco); Armando Ariza-Castolo (Departamento de Qumica, Cinvestav)

The CASE-3D approach to the determination of stereochemical configuration and conformation may often require of DFT computations for prediction of chemical shielding tensors or scalar couplings. These computations may easily become a bottleneck on the computational process. We present here our machine-learning approaches to the prediction of scalar couplings, namely geminal 2JHH and 2JHC and vicinal 3JHH and 3JHC ones. Molecular representations combined purely geometry parameters with electronic parameters. The performance of our ML algorithms matched, if not improved, that of known empirical equations while having a much broader degree of applicability. Delta approaches based on cheap DFT computations for the prediction of 13C isotropic shieldings and chemical shielding anisotropies will be also presented.

ThOI: Inorganic, Organic and Hybrid Materials (parallel session)
16:00 - 17:50, Nautilus

16:00-16:25 **Cation Chaos in Photovoltaic Materials**

Presenting Author: Vladimir Michaelis

Vladimir Michaelis (University of Alberta)

A global decarbonization strategy is urgently needed in order to shift from our dependency of legacy fossil fuels to clean and reliable energy generation and storage alternatives. From a sustainability perspective the new materials will require a chemical design focused on highly abundant and inexpensive elements. Hence, to balance the chemical and optical properties with desired function requires an understanding of microscopic structure at the atomic scale. Solid-state nuclear magnetic resonance (NMR) spectroscopy is answering this call, paving the way to understanding ion substitution, doping, dynamics, and more. This contributed presentation will discuss our groups recent advances in mixed-ion photovoltaic materials containing exotic NMR-active nuclei.

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16:25-16:45 **Charge Density Wave Order of the Kagome Superconductors AV3Sb5 (A=K, Rb, and Cs): Structural Studies using Single Crystal Angle-Dependent 51V NMR**

Presenting Author: Xiaoling Wang

Arneil P. Reyes (National High Magnetic Field Laboratory); Brenden Ortiz (University of California, Santa Barbara); Andrea Capa Salinas (University of California, Santa Barbara); Stephen Wilson (University of California, Santa Barbara); Xiaoling (Cocoa) Wang (California State University East Bay)

The newly discovered kagome metal family AV3Sb5 (A = K, Rb or Cs) have attracted widespread interest very recently in the field of condensed matter due to their rich physical phenomena including symmetry-breaking charge-density waves (CDWs) and superconductivity. The specific CDW order exhibits cation dependence, and the real component of CDW corresponds to a real space charge inhomogeneity and results in a superstructure deformation of the crystal lattice. For the first time, we applied 51V single crystal NMR experiments at cryogenic temperatures on the AV3Sb5 series with relative orientational dependence between the crystal coordinates and the magnetic fields, in order to investigate the structural evolution and patterns of structural deformations caused by CDW.

16:45-17:05 **Opportunities for Absolute Quantitative MAS NMR in chemical and pharmaceutical applications.**

Presenting Author: Eric Breynaert

Sambhu Radhakrishnan (NMRCoRe); Vinod C. Vinodchandran (NMRCoRe); Alysson Morais (NRMCoRe); Maarten Houlleberghs (NMRCoRe); Dirk Dom (NMRCoRe, KU Leuven); KArel Duericnkx (NRMCoRe); loes verheyden (COK-kat, KU Leuven); Eric Breynaert (NMRCoRe, KU Leuven)

Solid state NMR is largely used to characterize materials with respect to chemical composition and functionalities. NMR supersedes all other spectroscopies in determining relative amounts of individual components in complex mixtures, but absolute quantification has long remained challenge. This contribution demonstrates how standard addition combined with MASNMR enables determination of water or residual solvents in porous materials used in catalysis, adsorption or controlled release. This information is essential for catalytic or adsorption applications, to optimize production or to fulfil quality control requirements set by health and safety regulations. The method is further extended to absolute quantification of solvents in adsorption applications and to the determination of crystalline silica impurities in amorphous silica in the frame of REACH legislation.

17:05-17:25 **One- and Two- Dimensional Pure Isotropic Proton NMR Spectra in Solids using Deep Learning**

Presenting Author: Pinelopi Moutzouri

Pinelopi Moutzouri (EPFL); Manuel Cordova (EPFL); Bruno Simes De Almeida (EPFL); Daria Torodii (EPFL); Lyndon Emsley (EPFL)

We have recently suggested new approaches, relying on the combination of fast MAS and 2D correlations, to tackle the problem of resolution in 1H NMR of solids. These approaches yield pure isotropic proton (PIP) spectra that contain only isotropic shifts and provide the highest 1H NMR resolution available today in rigid solids. Here, we extend the PIP approach to a second dimension and obtain ultra-high resolution 1H-1H double-quantum / single-quantum (DQ/SQ) dipolar correlation spectra for samples of L-tyrosine hydrochloride and ampicillin. We obtain two-dimensional DQ/SQ spectra with significantly higher resolution as compared to DQ/SQ spectra acquired at 100 kHz MAS allowing the identification of resolved isotropic correlation peaks that were previously overlapped.

17:25-17:50 **Reaction mechanism of syngas conversion on bifunctional catalysts revealed by solid-state NMR spectroscopy**

Presenting Author: Guangjin Hou

Guangjin Hou (Dalian Institute of Chemical Physics)

Syngas (H2/CO) is one of the most important C1-chemistry platforms for the utilization of non-petroleum carbon resources such as natural gas, coal or shale gas. Recently, an increasing number of studies have demonstrated that the bifunctional catalyst concept of physically mixing metal oxides and zeolites (OXZEO) provides a promising alternative to go beyond the ASF limitation and tackle the selectivity challenge, but the active sites and underlying mechanism are not yet explored. Herein, we performed solid-state NMR spectroscopy to investigate the mechanism of the syngas conversion over these bifunctional catalysts, including the activation of syngas on the oxide surface, site-selective adsorption, the reaction intermediates, the first C-C bond formation, and the reaction routes in zeolite, etc.

Monterey Bay Aquarium Social Event
18:30-22:30
Adv. Purchase Ticket is Required! Ticket sales close Mon. April 17 at noon OR when sold-out. Don't be disappointed, please purchase your ticket ASAP!