

**52nd SouthEastern Magnetic
Resonance
Conference**
a SERMACS-2024 SYMPOSIUM

Hosted by the Georgia Institute of Technology
and Emory University,
October 24-26, 2024

Organizers:

ssNMR - Anant Paravastu, Georgia Institute of Technology (Chair)

ssNMR - Johannes (Hanno) Leisen, Georgia Institute of Technology

sNMR - Andrew McShan, Georgia Institute of Technology

sNMR - Hongwei Wu, Georgia Institute of Technology

MRI - David Reiter, Emory University

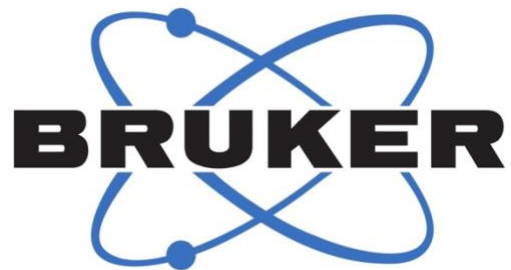
EPR - Kurt Warncke, Emory University

Venue:

AmericasMart Atlanta Convention Center

230 John Portman Blvd NW,
Atlanta, GA 30303

Sponsors of the 52nd SEMRC:



52nd SEMRC SYMPOSIUM AGENDA

Oral Presentation and other Events:

52nd SEMRC Starts on Thursday, October 24, 2024

Thursday, October 24th, 2024

Location X	ORAL SESSION: Biological MR 1 <i>Presiding: Andrew McShan, Georgia Institute of Technology</i>
8:30 AM – 8:40 AM	<i>Introductory Remarks from the Organizers</i>
8:40 AM – 9:20 AM	SEMRC Plenary Lecture: Ayyalusamy (Rams) Ramamoorthy , Florida State University and National High Magnetic Field Laboratory <i>Polymer and Peptide based Nanodiscs to Study Lipid Membranes by NMR Spectroscopy</i>
9:20 AM – 9:40 AM	Weimao Zhong , Georgia Institute of Technology <i>NMR-guided discovery, structural characterization, and biosynthesis of ureido peptidic natural products from marine Microbulbifer spp. bacteria</i>
9:40 AM – 10:00 AM	Tanveer Shaikh , Mississippi State University <i>Characterization of the complement C3dg protein using NMR spectroscopy</i>
10:00 AM – 10:20 AM	BREAK
10:20 AM – 11:00 AM	Sharon Campbell , University of North Carolina School of Medicine <i>Use of NMR in hybrid structural biology approaches to study RAS and heterotrimeric GTPases</i>
11:00 AM – 11:30 AM	Robert Silvers , Florida State University <i>Human La-Related Proteins and RNA Recognition</i>
11:30 AM – 12:00 PM	Jenny Yang , Georgia State University <i>Noninvasive Early Detection and Stage of Chronic Diseases with Precision MRI (pMRI)</i>
12:00 PM – 1:00 PM	LUNCH BREAK
Location X	ORAL SESSION: MR for Materials and Environment 1 <i>Presiding: XX, XX</i>
1:00 PM – 1:05 PM	<i>Opening Remarks</i>
1:05 PM – 1:35 PM	Yan-Yan Hu , Florida State University and National High Magnetic Field Laboratory <i>NMR/MRI studies of ion transport, interface chemistry, and dendrite formation in solid-state batteries</i>
1:35 PM – 1:55 PM	Leah Casabianca , Clemson University <i>NMR techniques for examining binding between small molecules and nanoparticles with environmental relevance</i>
1:55 PM – 2:15 PM	Zach Dowdell , Florida State University and National High Magnetic Field Laboratory <i>Mechanochemical syntheses of HCl salts and their structural characterization using ³⁵Cl solid-state NMR and dispersion-corrected DFT calculations</i>

2:15 PM – 2:35 PM	Sara Termos , Florida State University and National High Magnetic Field Laboratory <i>Exploration of wide-line and ultra-wide-line solid-state NMR spectroscopy of unresponsive transition metal nuclei: Challenges and insights</i>
2:35 PM – 2:55 PM	Mingyu Song and Hyun June Moon , Georgia Institute of Technology <i>Roles of Polyol Additives in Promoting CO₂ Capture in PEI/Silica Adsorbents</i>
2:55 PM – 3:10 PM	BREAK
3:10 PM – 3:40 PM	Alexey Silakov , Pennsylvania State University <i>EPR investigation of O₂-tolerant [FeFe] hydrogenases: towards sustainable H₂ production.</i>
3:40 PM – 4:00 PM	Martin Bakker , The University of Alabama <i>EPR studies of Phthalocyanines encapsulated in Zeolites</i>
4:00 PM – 4:20 PM	Kristen Aviles , Pennsylvania State University <i>Control over the electronic structure of alkanethiolate stabilized palladium nanoparticles revealed by conduction electron spin resonance and Evans method</i>
4:20 PM – 4:40 PM	Tanya Balandin , Georgia Institute of Technology <i>Magnetic characterization of open-shell narrow bandgap donor-acceptor conjugated polymers</i>

Friday, October 25th, 2024

Location X	ORAL SESSION: Biological MR 2 Presiding: XX, XX
8:30 AM – 8:35 AM	<i>Opening Remarks</i>
8:35 AM – 9:05 AM	Candace Fleischer , Emory University School of Medicine <i>In vivo MR thermometry and biophysical modeling of human brain temperature</i>
9:05 AM – 9:25 AM	Katie Whitcomb , Emory University <i>Comparative Analysis of the Dynamics of the Intrinsically Disordered Protein, α-Synuclein, in Monomer, Oligomer, and Fibril Forms, Under Controlled Confinement</i>
9:25 AM – 9:45 AM	Oluwabukola Bamishaye , Georgia State University <i>Early Detection of Invasive Lung Cancer and Multiorgan Metastasis Using Collagen-Targeted Protein MRI Contrast Agent</i>
9:45 AM – 10:05 AM	Thomas Manning , Valdosta State University <i>Role of FT-ICR and FT-NMR in Understanding the Medicinal Activity of a Novel Excipient for POX Viruses</i>
10:05 AM – 10:35 AM	Tatyana Smirnova , North Carolina State University <i>Local electrostatics of lipid-protein systems by spin labeling EPR</i>
10:35 AM – 10:55 AM	BREAK
	ORAL SESSION: MR for Materials and Environment 1 Presiding: XX, XX
10:55 AM – 11:15 AM	Alexander Nevzorov , North Carolina State University <i>Pulsed EPR/NMR/DNP Spectrometer Operating at 200 GHz/300 MHz</i>
11:15 AM – 11:35 AM	Carl Fleischer , Florida State University and National High Magnetic Field Laboratory <i>New Applications of Quadrupolar NMR Crystallography Guided Crystal Structure Prediction</i>
11:35 AM – 11:55 AM	Faith Scott , National High Magnetic Field Laboratory <i>DMSO-Sorbitol as a novel high temperature matrix for magic angle spinning-dynamic nuclear polarization nuclear magnetic resonance (MAS-DNP NMR)</i>
11:55 PM – 1:00 PM	LUNCH BREAK

Location X	ORAL SESSION: MR for Materials and Environment 2 Presiding: XX, XX
1:00 PM – 1:05 PM	<i>Remarks from the Organizers</i>
1:05 PM – 1:45 PM	SEMRC Plenary Lecture: Rob Schurko , Florida State University and National High Magnetic Field Laboratory <i>Ultra-wideline NMR spectroscopy and the crucial roles of protons</i>
1:45 PM – 2:05 PM	Marc Ter Horst , The University of North Carolina at Chapel Hill <i>LED NMR and azobenzene photoconversion</i>
2:05 PM – 2:25 PM	Robert Smith , Florida State University and National High Magnetic Field Laboratory <i>Solid-state NMR spectroscopy: a window into the properties of plasmonic semiconductor nanocrystals</i>
2:25 PM – 2:45 PM	H.N. Cheng , USDA Agricultural Research Service <i>Selected NMR Methodologies for Polymer Characterization</i>
2:45 PM – 3:05 PM	BREAK
	ORAL SESSION: Biological MR 3 Presiding: XX, XX
3:05 PM – 3:25 PM	Mia McMahon , Georgia State University <i>Development of a Highly Selective Dual-Purpose Theragnostic Agent for the Calcium Sensing Receptor</i>
3:25 PM – 3:55 PM	John Oshinski , Emory University <i>4D Flow MRI shows pro-thrombotic hemodynamics in patients with carotid webs</i>
3:55 PM – 4:25 PM	Thomas Leeper , Kennesaw State University <i>Inhibiting the inhibitor: NMR methods to obtain molecules that promote native endolytic activity in Pseudomonas aeruginosa.</i>
4:25 PM – 4:45 PM	Veronika Szalai , National Institute of Standards and Technology <i>Structure and dynamics of flexibly-linked, multi-domain proteins determined using spins, scattering, and simulations</i>

Saturday, October 26th, 2024

Location X	ORAL SESSION: Biological MR 4 Presiding: XX, XX
8:30 AM – 8:35 AM	<i>Opening Remarks</i>
8:35 AM – 8:55 AM	Alex Smirnov , North Carolina State University <i>Wet, Dry, or Frozen: Maintaining Macroscopic Alignment of Lipids in Nanoporous Substrates</i>
8:55 AM – 9:15 AM	Alicia Robang , Georgia Institute of Technology <i>Designing β-sheet peptide assemblies</i>
9:15 AM – 9:35 AM	Benjamin Wylie , Texas Tech University <i>Lipid Regulation of GPCR dynamics and Ligand-Receptor Association</i>
9:35 AM – 10:05 AM	Shella Keilholz , Emory and Georgia Institute of Technology <i>Towards multimodal imaging in awake, behaving mice</i>
10:05 AM – 10:25 AM	BREAK
10:25 AM – 10:55 AM	Fatemeh Adelnia , Vanderbilt University and Vanderbilt University Medical Center <i>In vivo Tissue Characterization by R1ρ Dispersion Imaging</i>
10:55 AM – 11:25 AM	Mark dela Cerna , Georgia Southern University <i>Identification of inhibitors and binders of the oncogenic phosphatase of regenerating liver 3 (PRL3/PTP4A3)</i>
11:25 AM – 11:45 AM	Anant Paravastu , Georgia Institute of Technology <i>How Proteins or Peptides Could Aggregate without Forming Canonical Amyloid Fibrils</i>

11:45 AM – 12:05 PM	Francis Akinlotan , Georgia State University <i>Noninvasive Visualization of Molecular Signatures of Liver Fibrosis Progression by Collagen Targeted Protein MRI Contrast Agent</i>
12:05 PM – 1:05 PM	LUNCH BREAK
Location X	ORAL SESSION: MR for Materials and Environment 3 Presiding: XX, XX
1:05 PM – 1:35 PM	Martin Mourigal , Georgia Institute of Technology <i>Cryogenic platform to investigate strong microwave cavity-spin coupling in correlated magnetic materials</i>
1:35 PM – 1:55 PM	Thomas Devore , James Madison University <i>NMR belongs in the physical chemistry laboratory</i>
1:55 PM – 2:15 PM	Jakub Hruby , National High Magnetic Field Laboratory <i>Identification of an X-Band Clock Transition in Cp'3Pr– Enabled by a 4f25d1 Configuration</i>
2:15 PM – 2:35 PM	Johan van Tol , Florida State University <i>Relaxation of Nitrogen Donors in Silicon Carbide at High Magnetic Fields</i>
2:35 PM – 2:55 PM	Florian Ressnik , Georgia Institute of Technology <i>VT and EXSY NMR analysis of ligand exchange barriers in actinide inverse trans influence complexes</i>
2:55 PM – 3:05 PM	<i>Closing Remarks</i>
3:05 PM – 3:45 PM	<i>Business Meeting</i>

52nd SEMRC SYMPOSIUM POSTER SESSION
OCTOBER 25 (FRIDAY) EVENING
Location XX:
Poster Board Assignments TBA

1. Protein-coupled solvent dynamics in fibrillar amyloid- β (1-42) under controlled confinement revealed by using electron paramagnetic resonance spectroscopy. **Hana Alsheikh**, Emory University
2. Observing multi-photon charge carrier spin transitions between Floquet states in organic light-emitting diodes. **Sabastian Atwood**, National High Magnetic Field Laboratory & University of Utah
3. Developing Chemical Probes for PRL3 by Fragment-Based Drug Discovery and Protein-Observed Fluorine (ProF) NMR. **Grace Bennett**, Georgia Southern University
4. Solution characterization of a high-valent complex of 141Pr. **Andrew Boggiano**, Georgia Institute of Technology
5. Analytical measure of mean distance and uncertainty in Double Electron Electron Resonance. **Michael Bowman**, The University of Alabama
6. Solid-state NMR and X-ray crystallography studies of rippled sheet peptide assemblies. **Tzu-Ying Chiu**, Georgia Institute of Technology
7. Monitoring accelerated aging reactions with powder X-ray diffraction and 113Cd solid-state NMR spectroscopy. **James Cohan**, Florida State University & National High Magnetic Field Laboratory

8. Small molecule characterization of ^{13}C enriched duckweed *Spirodela polyrhiza*. **Stephanann Costello**, University of Georgia
9. ^{19}F NMR study of binding between functionalized polystyrene nanoparticles and perfluorooctanoic acid (PFOA). **Sekinah Dauda**, Clemson University
10. Exploring the effect of Mn^{2+} on cyclic GMP-AMP synthase activity. **Eric Dey**, Samford University
11. Combining Solid-State NMR and Cryo-EM to Probe Structure of Designer α -Helical Filament. **Daniel Manogaran Dinakarapandian**, Georgia Institute of Technology
12. Development and characterization of hProCA32.Collagen1: A novel protein-based MRI contrast agent for enhanced liver disease diagnosis. **Farzaneh Dorabadizare**, Georgia State University
13. BOLD imaging as a non-invasive biomarker for microvascular reactivity in Diabetic Foot Ulcers. **Scott Edwards**, Emory University School of Medicine,
14. Network for Advanced NMR and CCRC NMR Facility: Opportunities for Metabolomics and Studies of Biomolecules at Fields up to 1.1 GHz. **Alexander Eletsy**, University of Georgia
15. University of Georgia Complex Carbohydrate Research Center, Metabolite fraction libraries. **Christopher Esselman**, University of Georgia
16. Magnetic resonance studies of carotenoid radicals and complexes. **Alexandrina Focsan**, Valdosta State University
17. Protein-coupled solvent dynamics of anti-aggregative small-molecule interaction with α -synuclein. **Shady Fouad**, Emory University,
18. High-field continuous-wave EPR and FIRMS investigation of spin state transitions in Schiff base metalorganic Mn^{3+} complexes. **Brittany Grimm**, Florida State University & National High Magnetic Field Laboratory
19. Experimental and computational advances in solid-state NMR spectroscopy of the platinum group elements. **Sean Holmes**, Florida State University & National High Magnetic Field Laboratory
20. β -sheet co-assembly interactions guide organization of charged peptide-polydiacetylene conjugates. **Jeffrey Li**, Georgia Institute of Technology
21. Quantification of NMR Relaxometry Data with Machine Learning. **Shinjer Li**, William & Mary
22. Metal-oxide nanoparticles alter photoinitiated degradation products in oil lubricants: Spin trapping EPR studies. **Julie Matheny**, NC State University
23. Assessing surface electrostatics of lipid bilayers from molecular motion of EPR probes. **Ngan Nguyen**, NC State University,
24. High-field cavity-based EPR with in situ two-axis crystal rotation capability. **Quang Nguyen & Andrew Cook**, Florida State University & National High Magnetic Field Laboratory
25. Understanding the binding of amino acids to plastic nanoparticles in natural waterways using saturation-transfer difference (STD)-NMR. **Rajan Rai**, Clemson University
26. Acetone's abnormal relaxation time trend is a result of dissolved oxygen. **Patrick Randolph**, James Madison University,

- 27.** Tracing a pathway for detergent assisted oligomerization for A β 42. **Tarunya Rao Sudarshan**, Georgia Institute of Technology
- 28.** Solid gains: Creatine characterized by multinuclear Solid-State NMR. **Victoria Rash**, The University of Texas at Dallas School of Natural Sciences and Mathematics
- 29.** Quantitative blood oxygen level dependent (qBOLD) MRI of the pancreas during glucose stimulation in type 2 diabetes: Initial comparisons with beta cell function. **Ellie Ray**, Emory University & Georgia Institute of Technology
- 30.** Mechanochemical synthesis and multinuclear solid-state NMR spectroscopy of metal coordination polymers. **Jazmine Sanchez**, Florida State University & National High Magnetic Field Laboratory
- 31.** High-field EPR analysis of Co- and Fe-based metal complexes: Unraveling electronic and geometric properties. **Kavipriya Thangavel**, National High Magnetic Field Laboratory
- 32.** Charge-clustering induced fast ion conduction in 2LiX-GaF₃: A strategy for electrolyte design. **Erica Truong**, Florida State University
- 33.** High-field EPR study of Mn(acac)₃ and Mn(mesacac)₃ and assessment of coherence properties. **Ronghe Wang**, Florida State University & National High Magnetic Field Laboratory
- 34.** Resolving select protein and coupled solvent configurational fluctuation contributions to enzyme catalysis. **Kurt Warncke**, Emory University
- 35.** Using parametric modulations to model and locate border proximity signals in the human brain: An fMRI study. **Omar Zeid**, Georgia Institute of Technology