

SEMR Conference and Symposium Program

Thursday, October 24

- 4:00 - 8:00 PM Registration
- 6:00 - 8:00 PM **Mixer** - Crystal Coast Ballroom

Friday, September 25, Stejskal Symposium (free for all registered conference attendees) - Empire Ballroom, Salons D & E

- 8:00 AM - 4:00 PM Registration
- 8:00 - 8:40 AM **Continental Imperial Breakfast** (free for all registered and invited symposium and conference attendees) - Empire Ballroom, Salons A&B
- 8:45 AM **Introductory Remarks: Jeffrey White**, North Carolina State University, Symposium Chairman
- 8:45 - 9:45 AM **Plenary Lecture: Jacob Schaefer**, Washington University
Early CPMAS Experiments at Monsanto with Ed Stejskal
- 9:45 - 10:30 AM **Gary Maciel**, Colorado State University
Adventures with Spins on the Surface of Silica
- 10:30 - 10:45 AM **Coffee Break** - Empire Ballroom, Salons A & B
- 10:45 - 11:30 AM **Charles Johnson**, University of North Carolina - Chapel Hill
A Celebration of the Stejskal-Tanner Equation and Its Legacy
- 11:30 - 12:15 PM **Dan Raftery**, Purdue University
Sensitivity and Throughput Improvements in NMR Spectroscopy
- 12:15 - 1:15 PM **Buffet Lunch** (free for all registered and invited symposium and conference attendees) - Empire Ballroom, Salons A & B
- 1:15 - 2:15 PM **Plenary Lecture: Alex Pines**, University of California - Berkeley
NMR at Variable Distances and Angles
- 2:15 - 3:00 PM **Edward Samulski**, University of North Carolina - Chapel Hill
Biaxial Deformation of Polymer Networks and Deuteron Quadrupolar Interactions
- 3:00 - 3:15 PM **Coffee Break** - Empire Ballroom, Salons A & B
- 3:15 - 4:00 PM **Alan English**, DuPont Central Research & Development
Polytetrafluoroethylene: Synthesis, Structure, Dynamics, and Processing

- 4:00 - 4:45 PM **Dave Cory**, Massachusetts Institute of Technology
NMR Perspectives on the Physics of Quantum Information Processing
- 4:45 - 5:30 PM **Alan Tonelli**, North Carolina State University
NMR Studies of Polymers Included in and Coalesced from Their Inclusion Compounds Formed with Host Cyclodextrins
- 7:00 - 9:00 PM **Reception and Banquet in Honor of E.O. Stejskal** (separate registration and fee of \$30 required) - Crystal Coast Ballroom

Saturday, October 26, SEMRC - Empire Ballroom, Salons D & E

- 8:00 - 8:30 AM **Continental Imperial Breakfast** (included with registration fee) - Empire Ballroom, Salons A & B
- 8:30 - 8:40 AM **Opening remarks: Alex Smirnov and Tatyana Smirnova**, North Carolina State University, SEMRC Co-Chairs

Magnetic Resonance in Biology and Medicine

Chair: Kurt Warncke, Emory University

- 8:40 - 9:20 AM **Plenary Lecture: David D. Thomas**, University of Minnesota
A Coordinated EPR and NMR Analysis of Membrane Protein Structure and Dynamics
- 9:20 - 9:40 AM **The Nuclease A Inhibitor Represents a New Variation of the Rare PR-1 Fold**
Geoffrey A. Mueller, Thomas W. Kirby, Eugene F. DeRose, Mark S. Lebetkin, Gregor Meiss, Alfred Pingoud, and Robert E. London
National Institute of Environmental Health Sciences, Institut für Biochemie, Justus-Liebig-Universität Heinrich-Buff-Ring Giessen, Germany
- 9:40 - 10:00 AM **PISA Wheel Helical Rotational Angle Analysis of M2 Proton Channel from Influenza A Virus**
Changlin Tian, Jun Hu and Timothy A. Cross
National High Magnetic Field Laboratory, Institute of Molecular Biophysics, Florida State University
- 10:00 - 10:20 AM **Coffee Break** - Empire Ballroom, Salons A & B

Magnetic Resonance in Biology and Medicine

Chair: John Cavanagh, North Carolina State University

- 10:20 - 10:40 AM **High Resolution Magnetic Relaxation Spectroscopy**
Robert G. Bryant, Ching-Ling Teng, Kenneth G. Victor, Galina Diakova, Alexandra Van Quynh, Jean-Pierre Korb, Jack Freed, Alex Nevzorov, and Shawn Wagner
University of Virginia Charlottesville, Laboratoire de Physique de la Matière Condensée, Palaiseau, France, Cornell University
- 10:40 - 11:00 AM **Structure of the Intact Stem and Bulge of HIV-1 Ψ -RNA Stem Loop SL1**
Dana C. Lawrence, Carrie C. Stover, Jennifer Noznitsky, Zhengrong Wu, and Michael F. Summers
Howard Hughes Medical Institute and Department of Chemistry and Biochemistry, University of Maryland, National Institutes of Health
- 11:00 - 11:20 AM **Variable Field EPR Studies of Radicals Formed During the Oxidation of Myoglobin by Hydrogen Peroxide**
Tatyana. A. Konovalova, and L. D. Kispert
University of Alabama
- 11:20- 11:40 AM **Orientation-Selection ESEEM Spectroscopy Reveals the Geometry of Reactant Centers in the Co^{II} -Substrate and Product Radical Pair States of Coenzyme B_{12} -Dependent Ethanolamine Deaminase**
Kurt Warncke, and Jeffrey M. Canfield
Emory University
- 11:40 - 12:00 PM **Structural Basis for Topoisomerase I Inhibition by Nucleoside Analogs** William H. Gmeiner, Xi-an Mao, Shuyuan Yu, Richard T. Pon, Phillipe Pourquier, and Yves Pommier
Wake Forest University School of Medicine, Core DNA Synthesis Facility, University of Calgary, Alberta, Canada, Laboratoire de Pharmacologie des Agents Anticancéreux, Institut Bergonie, Bordeaux, France, National Institutes of Health
- 12:00 - 1:15 PM **Buffet Lunch** (included with registration fee) - Empire Ballroom, Salons A & B

Magnetic Resonance in Biology and Medicine

Chair: William H. Gmeiner, Wake Forest University School of Medicine

- 1:15 - 1:55 PM **Plenary Lecture: Balaraman [Raman] Kalyanaraman**,
Medical College of Wisconsin
Bicarbonate-Dependent Peroxidase Activity of Human Cu, Zn SOD Causes Aggregation of Protein: Role of Tryptophan-Derived Radical Reaction

- 1:55 - 2:15 PM ***Metals and Proteins: A Double Edged Sword***
John Cavanagh
NC State University
- 2:15- 2:35 PM ***Q-band (34 GHz) EPR Characterization of the “g=4.1 Signal” from the S₂ State of the Photosynthetic Oxygen Evolving Complex***
Alice Haddy, K. V. Lakshmi, Gary W. Brudvig, and Harry A. Frank
University of North Carolina -Greensboro, Yale University, University of Connecticut
- 2:35 - 2:55 PM ***EPR Spectroscopy Studies on the Structural Transition of Nitrosyl Hemoglobin in the Arterial-Venous Cycle of DEANO-Treated Rats***
Adrian R. Jaszewski, Yang C. Fann, Yeong-Renn Chen, Keizo Sato, Jean Corbett, and Ronald P. Mason
National Institute of Environmental Health Sciences
- 2:55 - 3:15 PM **Coffee Break** - Empire Ballroom, Salons A & B
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- Magnetic Resonance in Physics and Material Science**
Chair: Haskell W. Beckham, Georgia Institute of Technology
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- 3:15 - 3:35 PM ***Enhanced Sensitivity Magnetic Resonance Techniques for Semiconductors: Optical Pumping, Dynamic Nuclear Polarization, and Electrical Detection***
Clifford R. Bowers,
National High Magnetic Field Laboratory, University of Florida
- 3:35 - 3:55 PM ***9-287 GHz EPR Study of Fe-MCM-41 Molecular Sieves***
Lowell D. Kispert, T. A. Konovalova, J. van Tol, and L. C. Brunel
University of Alabama, National High Magnetic Field Laboratory, Florida State University
- 3:55 - 4:15 PM ***Evaluating Solid-State Structures for Quantum Computing: The Potential of High Frequency Electron Nuclear Double Resonance***
Louis C. Brunel, and J. van Tol
National High Magnetic Field Laboratory, Florida State University
- 4:15 - 4:35 PM ***Nuclear Spin Relaxation in Alkali Halide Single Crystals During Deformation***
K. Linga Murty, and O. Kanert
NC State University, National Science Foundation, Universitat Dortmund, Dortmund, Germany

- 4:35 - 4:55 PM **Studies of Counterion Binding to Cationic Micelles and Solloids Using X- band and W-band EPR**
Martin G. Bakker, Todd Morris, Edward L. Granger, and Alex I. Smirnov
The University of Alabama, College of Medicine, University of Illinois at Urbana, North Carolina State University
- 6:00 – 7:30 PM **Buffet Dinner** (included with registration fee) - Empire Ballroom, Salons A, B, & C
- 6:00 – 9:00 PM **Poster Session** - Empire Ballroom, Salons A, B, & C

Sunday, October 27, SEMRC - Empire Ballroom, Salons D & E

- 8:00 - 8:30 AM **Breakfast Snack** (included with registration fee) - Empire Ballroom, Salons A & B

Novel Methods and Applications in Magnetic Resonance

Chair: Robert G. Bryant, University of Virginia

- 8:30 - 9:10 AM **Plenary Lecture: R. David Britt**, University of California - Davis
Pulsed EPR as a Probe of the Chemistry of Photosynthetic Oxygen Evolution
- 9:10 - 9:30 AM **Sorption Isotherm Measurements by NMR**
Haskell W. Beckham, and Johannes Leisen
Georgia Institute of Technology
- 9:30 - 9:50 AM **Production of >65% Nuclear Spin Polarized Xenon-129: Methods for Generation, Delivery, Collection, and Polarization Measurement in the Gaseous and Liquid States**
Bhavin B. Adhyaru, Anthony L. Zook, and Clifford R. Bowers
National High Magnetic Field Laboratory, University of Florida
- 9:50 - 10:10 AM **Coffee Break** - Empire Ballroom, Salons A & B

Novel Methods and Applications in Magnetic Resonance

Chair: Lowell D. Kispert, University of Alabama

- 10:10 - 10:30 AM **Effective Repeat Time Characterizes T1-weighting**
W. Thomas Dixon, Daniel J. Blezek, Paritosh J. Dhawale, and Mukesh G. Harisinghani
General Electric Global Research, Department of Radiology, Massachusetts General Hospital

- 10:30 - 10:50 AM ***Excited Triplet States Studied by High-Frequency EPR: What Can We Learn?***
Johan van Tol, M. Bortolus, and L.C. Brunel
Center for Interdisciplinary Magnetic Resonance, National High Magnetic Field Laboratory, Florida State University
- 10:50 - 11:10 AM ***2D-FT-ESR in the mm-wave Age***
Keith Earle, Wulf Hofbauer, Curt Dunnam, and Jack Freed
Cornell University
- 11:10 - 11:30 AM ***Progress Toward Micron-Scale BOOMERANG NMR, and an Ideal Rodlike Liquid Crystal at High-Temperatures: Swimming Against the Mainstream***
Louis A. Madsen, Garrett M. Leskowitz, Daniel E. Miller, Kyung-Ah Son, Weilong Tang, Thomas George, Daniel P. Weitekamp, Theo J. Dingemans, and Edward T. Samulski
A. A. Noyes Laboratory of Chemical Physics Microdevices Laboratory at NASA-JPL, California Institute of Technology, University of North Carolina -Chapel Hill
- 11:30 - 11:50 AM ***The First Example of High-Frequency EPR Utilization in Identifying Ligand vs. Metal Oxidation in a Metal-Metal Bonded Complex: Cr₂(DPPC)₄PF₆***
Chris Ramsey, Naresh Dalal, F. Albert Cotton, and Penglin Huang
Florida State University, Texas A&M University
- 11:50 AM Brief Business Meeting to Plan Next SEMRC
- Conference Adjourn