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**  
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

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<th>Time</th>
<th>Session Title</th>
<th>Authors</th>
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<tr>
<td>10:20 - 10:40 AM</td>
<td>High Resolution Magnetic Relaxation Spectroscopy</td>
<td>Robert G. Bryant, Ching-Ling Teng, Kenneth G. Victor, Galina Diakova,</td>
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<td>Alexandra Van Quynh, Jean-Pierre Korb, Jack Freed, Alex Nevzorov,</td>
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<td>and Shawn Wagner</td>
<td>University of Virginia Charlottesville, Laboratoire de Physique de la</td>
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<td>Matière Condensée, Palaiseau, France, Cornell University</td>
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<td>10:40 - 11:00 AM</td>
<td>Structure of the Intact Stem and Bulge of HIV-1 Ψ-RNA Stem Loop SL1</td>
<td>Dana C. Lawrence, Carrie C. Stover, Jennifer Noznitsky, Zhengrong Wu,</td>
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<td>and Michael F. Summers</td>
<td>Howard Hughes Medical Institute and Department of Chemistry and Biochemistry,</td>
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<td>University of Maryland, National Institutes of Health</td>
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<td>11:00 - 11:20 AM</td>
<td>Variable Field EPR Studies of Radicals Formed During the Oxidation of Myoglobin</td>
<td>Tatyana. A. Konovalova, and L. D. Kispert</td>
<td>University of Alabama</td>
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<td>by Hydrogen Peroxide</td>
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<td>11:20 - 11:40 AM</td>
<td>Orientation-Selection ESEEM Spectroscopy Reveals the Geometry</td>
<td>Kurt Warncke, and Jeffrey M. Canfield</td>
<td>Emory University</td>
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<td>of Reactant Centers in the Co²⁻-Substrate and Product Radical Pair States</td>
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<td>of Coenzyme B₁₂⁻-Dependent Ethanolamine Deaminase</td>
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<td>11:40 - 12:00 PM</td>
<td>Structural Basis for Topoisomerase I Inhibition by Nucleoside Analogs</td>
<td>William H. Gmeiner, Xi-an Mao, Shuyuan Yu, Richard T. Pon,</td>
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<td>Phillipe Pourquier, and Yves Pommier</td>
<td>Wake Forest University School of Medicine, Core DNA Synthesis</td>
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<td>Facility, University of Calgary, Alberta, Canada, Laboratoire de Pharmacologie des Agents</td>
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<td>Anticancereux, Institut Bergonie, Bordeaux, France, National Institutes of Health</td>
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<td>12:00 - 1:15 PM</td>
<td>Buffet Lunch (included with registration fee)</td>
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<td>Empire Ballroom, Salons A &amp; B</td>
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## Magnetic Resonance in Biology and Medicine
Chair: William H. Gmeiner, Wake Forest University School of Medicine

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

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  
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

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**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

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**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**  
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: $\text{Cr}_2(\text{DPPC})_4\text{PF}_6$**  
*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