31th International EPR Symposium Preliminary Program
July 27 – 31, 2008
Beaver Run Resort, Breckenridge, Colorado

2008 EPR Symposium organizing committee: *Hassane S. Mchaourab, Chair. Yeon-Kyun Shin, Neil Hogg, Peter Doan, Brian Bennett, Alex Angerhofer, Eduardo Perozo, Howard Halpern, Gunnar Jeschke, Glenn Millhauser.*

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• Sunday, July 27, 2008

1:30-4:30 pm Workshop: Quantitative EPR, Gareth Eaton and Dave Barr Chairing

5:00 pm : Bruker annual progress and products report (including appetizers and refreshments)

If you plan to attend the Workshop or the Bruker Presentation, please notify Art Heiss (ah@bruker.com) and Gareth Eaton (geaton@du.edu) so that we can arrange handouts and refreshments.

• Monday, July 28, 2008

Session I, Computational Methods for Protein Structure Determination using EPR Constraints, Eduardo Perozo, chairing

8:15 am	**Welcoming Remarks.** Hassane S Mchaourab
8:20	**Introduction to Session.** Eduardo Perozo
8:25	**Molecular Specialties lecture: De Novo High-Resolution Protein Structure Determination from Sparse Spin-Labeling EPR Data.** Jens Meiler, Vanderbilt University
8:50	**Refinement of molecular structure using restraints based on ESR data**. Benoit Roux, University of Chicago.
9:20	**Application of Structural Restraints Obtained by Site-Directed Spin Labeling to Protein Structure and Protein-Membrane Interactions.** David Cafiso, University of Virginia
9:45	**Structural origin of weakly ordered nitroxide motion in the R1 spin label side chain.** Mark Fleissner, University of California, Los Angeles
10:00	*Break*
10:20	**Computational modelling of DEER and cwEPR distances and their distributions.** Peter Fajer, Florida State University

10:45 **PKCα C2 Domain: Use of EPR Depth Parameters and Modeling to Define the Membrane Docking Geometries of Two Membrane-bound States.** Joe Falke, University of Colorado.

11:10 **Gating-related Conformational Changes in the Outer Vestibule of KcsA: A Functional and Spectroscopic Analysis**. H. Raghuraman, University of Chicago, Julio F. Cordero-Morales, Eduardo Perozo, The University of Chicago

11:25 **Spin label dynamics as a probe of the force-generating region in muscle and nonmuscle myosin II.** Yuri E. Nesmelov, Roman V. Agafonov, Margaret A. Titus, David D. Thomas, University of Minnesota.

11:40 **Double Electron-Electron Resonance Measurements on the Flap Region of Drug-Resistant HIV-1 Protease Variants**. Gail E. Fanucci, University of Florida.

12:00 Lunch – buffet included in registration fee

Session II, Joint EPR/NMR session: Spins in ordered aggregates: What magnetic resonance tells us about amyloids and neurodegenerative disease.

1:30 pm **Dipole Recoupling and Dynamic Nuclear Polarization at High Magnetic Fields.** Robert Griffin, MIT.

2:00 **Amyloid Protein Structure and Membrane Interaction Studied by Site-Directed Spin labeling.** Ralf Langen, University of Southern California.

2:30 **Solid-State NMR of Amyloid Aggregates and Paramagnetic Systems.** Yoshitaka Ishii, University of Illinois at Chicago

3:00 **The Interaction of the A-beta amyloid peptide and apolipoprotein E examined by spin-labeled side chains.** John C. Voss, University of California Davis.

3:30 *Break*

4:00 **Solid-State NMR of Unfolded and Misfolded Proteins: Methods and Results.** Robert Tycko, NIH

4:30 **Molecular Architecture of Human Prion Protein Amyloid: A Spin Labeling and H/D Exchange Study.** Witold K. Surewicz. Case Western Reserve University.

5:00 – 7:00 Conference Reception and Mixer
7:30 – 9:30 pm, Session III, Posters,

- **Tuesday, July 29, 2008**

Session IV, Modern Approaches to Spin Trapping, Neil Hogg Chairing

8:30 am **Detection of Protein and DNA Free Radicals in Organelles, Cells, and Tissues.** Ronald P. Mason NIEHS/NIH

9:05 **Spin Trapping of Nitric Oxide in Biomedical Applications,** Jay Zweier. The Ohio State University

9:40 **Rationally Improving Isoniazid Activity: Better TB drugs from Spin Trapping** Graham Timmins, University of New Mexico

10:10 Break

10:30 **Mass Spectrometric Characterization of Protein Radical Adducts Induced by Oxidative Damage.** Leesa J. Deterding NIEHS/NIH

11:00 **Tetrahydrobiopterin as a target of Mn(III) *ortho* tetrakis *N*-ethylpyridylporphyrin, MnTE-2-PyP^{5+}, actions in mice model of breast tumor** Jeanette Vasquez –Vivar, Medical College of Wisconsin.

11:30 **p-Nitrostilbene-t-butyl-nitrone, a Novel Fluorescent Spin Trap for the Detection of ROS With Subcellular Resolution** Stefan Hauck, Yvonne Lorat and Wolfgang E. Trommer, Technical University Kaiserslautern

12:00 Lunch – buffet included in registration fee

Workshop on Pulse Dipolar EPR/DEER Data Analysis, Gunnar Jeschke Chairing

2:00 pm **TBA**, Jack H. Freed, Cornell University
2:25 **Pitfalls in DEER data analysis**. Gunnar Jeschke, ETH Zürich
2:50 **TBA**, Peter Fajer, Florida State University
3:15 **Moderated discussion and analysis of user data**, Moderator: Eric J. Hustedt, Vanderbilt University

Session V, Recognition of Gareth and Sandra Eaton Service
4:15 **Introduction by Jim Hyde**
4:30 **The EPR Symposium and the Evolution of Modern EPR**, Gareth and Sandy Eaton
5:00 – 7:00 Reception and Light Dinner

Session VI, Lawrence H. Piette Memorial Lecture
7:00 **Introduction to Lawrence H. Piette Memorial Lecture**
7:05 **2008 Lawrence H. Piette Memorial Lecture – EPR in Hemolytic Disorders: Cell-Free Hemoglobin, Oxidative Stress and the Bioavailability of Nitric Oxide.**
Neil Hogg, Medical College of Wisconsin

7:45 – 9:45 pm Session VII, Posters,

- ## Wednesday, July 30, 2008

Session VIII, Biomechanisms and Metallomolecules, Brian Bennett and Peter Doan Chairing
8.10 am **Introductory Remarks by Brian Bennett and Peter Doan**
8.15 **Going to Extremes to Understand B12 Enyzme Catalysis by using EPR Spectroscopy.** Kurt Warncke, Emory University
8.40 **High-Frequency and –Field EPR Spectroscopy of High-Spin Transition Metal Complexes: Newest Developments.** Joshua Telser*, Roosevelt University
9.05 **Integrated Paramagnetic Resonance of High-Spin Co(II) in Biomimetic Environments.** David L. Tierney, University of New Mexico
9.30 **Using EPR Spectroscopy to Probe the Reaction Mechanism of Metallo-β-lactamases.** Michael W. Crowder, Miami University, OH
10.00 *Break*
10.30 **A triple resonance hyperfine sublevel correlation experiment for assignment of electron-nuclear double resonance lines.** Alexey Popatov*, Weizmann Institute of Science, Israel
10.50 **Quantitative EPR Spectroscopy of the Catalytic Cycle of Mn Dioxygenase.** Michael Hendrich, Carnegie Mellon University
11.15 **Analyzing Metal-RNA Interactions in Ribozymes Using EPR Methods.** Victoria J. DeRose, University of Oregon
11.40 **Analysis of Methylbenzylamine Stereoselectivity by a Chiral Copper System.** Ignacio Caretti, University of Antwerp, Belgium

12:00 Lunch – buffet included in registration fee

Session IX, EPR Imaging, Howard Halpern Chairing

1:30 pm **The Perspective of 250 MHz Electron Spin Echo Oxygen Imaging for Biomedical Applications.** Boris Epel, University of Chicago, Department of Radiation Oncology.

1:55 **Reconstruction of Rapid Scan EPR Images by Regularized Optimization.** Mark Tseitlin,[a,b] Tomasz Czechowski,[a] Gareth R. Eaton,[a] and Sandra S. Eaton,[a] [a]Department of Chemistry and Biochemistry, University of Denver and [b]Kazan Physical-Technical Institute of Russian Academy of Sciences, Kazan, Russia.

2:20 **Time-Domain and CW EPR Imaging: Some Recent Results.** S. Subramanian, S. Matsumoto, N. Devasahayam & M. C. Krishna, NCI, National Institutes of Health,

2:45 **Break**

Session X, Young Investigators, Hassane Mchaourab Chairing .

3:30 pm **Quenching Spin Decoherence in Diamond using 240 GHz EPR**. Susumu Takahashi, UC Santa Barbara

3: 45 **DEER as a Tool for the Conformational Characterization of Weak Protein-Protein Complexes and Self-Assembled Organic Structures.** J.E. Banham*, CAESR, Oxford, UK

4:00 **Overhauser spectroscopy of water as a new approach to study protein aggregation kinetics and membrane's fluid dynamics.** Songi Han, UCSB.

4:15 **1D and 2D Spectral-Spatial EPR Imaging of Dose Distribution: A Potassium Dithionate Dosimeter Following Irradiation with a C^{6+} beam.** H. Gustafsson*,[1] Krzysztof Kruczala,[2] Eva Lund,[1] and Shulamith Schlick,[3] [1]Linköping University, Sweden; [2]Jagiellonian University, Poland; [3]University of Detroit Mercy

4:30 **ESR Spin Probe Measurement of Structural Morphology and Local Probe Environment in a Nafion® Membrane Ion Exchanged with Multivalent Ions: Effects of Methanol.** Jamie S. Lawton, David E. Budil, Northeastern University.

5:00 General Business Meeting, Selection of the organizing committee for 2009.

• Thursday, July 31, 2008

Session XI, Material Sciences/ Instrumentation, Alex Angerhofer Chairing

8:10am **Single-Molecule Magnets**. Stephen Hill, University of Florida.

8:40 **Fourier Transform THz EPR on single molecular magnets.** Robert Bittl, Freie Universität Berlin.

9:10 **High-field ESR in low dimensional spin systems.** Sergei Zvyagin. Forschungszentrum Rossendorf.

9:40 **Low temperature high sensitivity magnetic resonance force microscopy.** Tim Mewes, University of Alabama.

10:10 **Break**

10:30 **Photocatalytic Properties of C_{60}- and TiO_2-based Nano-engineered Materials: EPR, NIR, and Single-cell-level AFM Assays.** Andrzej Sienkiewicz, Ecole Polytechnique Fédérale de Lausanne.

11:50 **Electrically Detected Magnetic Resonance Spectroscopy of Phosphorus Doped Crystalline Silicon at Very High Magnetic Fields ($B_0 \approx 8.5$T).** Christoph Boehme, University of Utah.

11:10 **Solid state quantum memory using the ^{31}P nuclear spin**. Brendon Lovett, Oxford University

11:30 **Development of Slot Array Resonator (SAR) for Pulsed EPR Spectrometer at Q-Band.** Mitsuhiro Ono, Yamagata University.

11:45 **Probing the Wavefunction of Nitrogen Shallow Donors in SiC by 240 GHz Pulsed EPR/ENDOR.** Johan van Tol, NHMFL.

* Recipient of a travel award.