



**41st INTERNATIONAL EPR SYMPOSIUM
JULY 22-27, 2018
SNOWBIRD, UTAH, USA**

EPR SYMPOSIUM COMMITTEE

Stefan Stoll (Chair)
Susumu Takahashi (Co-Chair 2018, Chair 2019)
Ania Bleszynski-Jayich
Christoph Boehme
Enrica Bordignon
Boris Epel
Gail Fanucci
Songi Han
Stephen Hill
Dane McCamey
John McCracken

AGENDA

SUNDAY, JULY 22, 2018

Pre-Conference Activities	
6:30-10:00 PM	Bruker EPR Users' Meeting <i>Meeting followed by Mixer</i>

MONDAY, JULY 23, 2018

8:10 AM	Welcoming Remarks. Stefan Stoll, EPR Symposium Chair
Session I: Biomacromolecules I. John McCracken, Chair	
8:15 AM	EPR Spectroscopy Reveals Protein Allostery and Signaling in a Bacterial Outer-membrane Transport Family. David S. Cafiso, University of Virginia
8:45 AM	PELDOR/DEER Spectroscopy Reveals Two Defined States of a Sialic Acid TRAP Transporter Substrate Binding Protein in Solution. Gregor Hagelueken, University of Bonn
9:00 AM	ESR Identification of Microtubule-binding Domain in Tau Protein. Timothée Chauviré, Cornell University
9:15 AM	EPR Distance Restraints as Core for Integrative Structure Modelling of 85 kDa PBTP1/EMCV- IRES Complex. Christoph Gmeiner, ETH Zürich
9:30 AM	A New Gadolinium Spin Label Gives High Sensitivity and Precision in Double Electron Electron Resonance Distance Measurements. Anokhi Shah, University of St Andrews
9:45 AM	<i>Break</i>
Session II: Biomacromolecules II. Gail Fanucci, Chair	
10:25 AM	Structural Dynamics of Desensitization in a Pentameric Ligand Gated Ion Channel. Sudha Chakrapani, Case Western Reserve University
10:55 AM	Light-induced Conformational Changes in Nitroxide-labeled Proteorhodopsin Detected by Time-resolved 240 GHz EPR at Room Temperature. C. Blake Wilson, University of California Santa Barbara
11:10 AM	Transporter Conformational Dynamics from Spin Labeling EPR Spectroscopy. Hassane S. Mchaourab, Vanderbilt University
11:40 AM	Non-nucleoside Inhibitors Modulate the Conformational States of the Finger and Thumb Subdomains of HIV-1 Reverse Transcriptase as Probed by Q-Band EPR Spectroscopy. Thomas Schmidt, National Institutes of Health
12:00 PM	<i>Lunch (included with registration)</i>
Session III: Spin Centers in Chemistry and Biology I. John McCracken, Chair	
1:30 PM	Histidine Handoff in the Prion Protein: New Cu²⁺Coordination Features for Protecting Against Neurodegeneration? Glenn Millhauser, University of California Santa Cruz
2:00 PM	Effect of Silica Support on Electrostatics of Lipid Interfaces in Nano-Bio Hybrid Systems. Tatyana I. Smirnova, North Carolina State University
2:15 PM	Lipoxygenase H-tunneling Efficiency Linked to ENDOR-detected Perturbations in Ground-state Structure. Ajay Sharma, Northwestern University
2:30 PM	2D-Related Hyperfine Spectroscopy on a Tetracycline-binding RNA Aptamer. Thilo Hetzke, Goethe University
2:45 PM	EPR Spectroscopy of Spin Probe, Label, and Time-Resolved, Reaction-Intrinsic Radicals Reveals Contributions of Specific Configurational Fluctuations and Solvent Coupling to the Core Chemical Step in Ethanolamine Ammonia-Lyase Catalysis. Kurt Warncke, Emory University
3:00 PM	<i>Break</i>
Session IV: Spin Centers in Chemistry and Biology II. Stephen Hill, Chair	
3:40 PM	Vanadyl Complexes: From Qubit Design to Quantum Simulation. Roberta Sessoli, University of Florence
4:10 PM	Endohedral Fullerenes as Molecular Qubits. ShangDa Jiang, Peking University
4:25 PM	Quantum Coherence Studies in Actinide and Lanthanide Organometallic Complexes. Floriana Tuna, University of Manchester
4:55 PM	Application of EPR Towards Cr/PNP Based Ethylene Tetramerization Catalysis. Sonia Chhabra, University of St Andrews
5:30-7:00 PM	<i>Conference Reception (included with registration)</i>
Session V: Posters	
7:30-9:00 PM	Authors Present for Posters Labeled A

Session VI: Spin Devices I. Ania Bleszynski-Jayich, Chair	
8:15 AM	Spin and Orbital Resonance Driven by a Mechanical Resonator. Gregory D. Fuchs, Cornell University
8:45 AM	Picoliter Diamond NMR. Victor M. Acosta, University of New Mexico
9:00 AM	Locking and Tracking Magnetic Resonance Spectra of NV⁻ Center for Real-time Magnetometry. Kapildeb Ambal, National Institute of Standards and Technology
9:15 AM	Precise Determination of Spin Concentration using Double Electron-electron Resonance. Susumu Takahashi, University of Southern California
9:30 AM	Electrical Detection of Charge Carrier Magnetic Resonance in the Strong Driving Field Limit When $B_1 \sim B_0$. Shirin Jamali, University of Utah
9:45 AM	<i>Break</i>
Session VII: Spin Devices II. Susumu Takahashi, Chair	
10:25 AM	EPR-on-a-chip – Current Trends and Future Research Directions. Jens Anders, University of Stuttgart
10:55 AM	Nanoscale EPR of Nitroxide Radicals using a NV Center in Diamond. Laura Mugica, University of Southern California
11:10 AM	Nanoscale NMR Enabled by Diamond Colour Centres. Fedor Jelezko, Ulm University
11:40 AM	Electron Spin Resonance of Individual Magnetic Atoms on Surfaces. Taeyoung_Choi, Ewha Womans University
12:00 PM	<i>Lunch (included with registration)</i>
Session VIII: Materials. Christoph Boehme, Chair	
1:30 PM	Charge Carrier Separation and Spin-Coupling in Photoactive Materials. Uwe Gerstmann, University of Paderborn
1:45 PM	Highly Efficient Optical Pumping of Spin Defects in Silicon Carbide for Stimulated Microwave Emission. Andreas Sperlich, University of Würzburg
2:00 PM	Spin-orbit Coupling Effects on Charge Carriers in Conjugated Polymers. Hans Malissa, University of Utah
2:15 PM	Light-induced Charge Separation in Polymer-Fullerene Organic Photovoltaics Studied by Multifrequency EPR and DFT. Jens Niklas, Argonne National Laboratory
2:30 PM	Electronic Structure Investigation of Self-doped type Organic Conductors by Magnetic Resonance Spectroscopy. Toshikazu Nakamura, Institute for Molecular Science
2:45 PM	Tuning Effective Charge Carrier Hyperfine Field Strengths in PEDOT:PSS Thin Films by Doping. Mandefro Teferi, University of Utah
3:00 PM	<i>Break</i>
Session IX: Other Topics. Stefan Stoll, Chair	
3:40 PM	A Bird's Eye View of the Chemical Compass - Magnetic Field Effects on the Photocycles of Cryptochrome. Christiane R. Timmel, University of Oxford
4:10 PM	Radiolysis Products at the Interface of Aluminum Oxyhydroxides and Strongly Basic Solutions. Eric Walter, Pacific Northwest National Laboratory
4:25 PM	Low Symmetry Orienting Potentials and Efficient Computation of ESR Line Shapes. Keith A. Earle, University at Albany
4:40 PM	Quantum Markovian Master Equation Approach to Magnetic Resonance: An Alternative to the Stochastic Liouville Equation. Jerryman A. Gyamfi, Scuola Normale Superiore di Pisa
Session X: Posters	
7:30-9:00 PM	Authors Present for Posters Labeled B

Session XI: Integrated Magnetic Resonance I. (Joint Session - EPR & SSNMR) Sophia Hayes & Gail Fanucci, Chairs	
8:05 AM	Time Domain Dynamic Nuclear Polarization (and Some CW Experiments on Proteins). Robert G. Griffin, Massachusetts Institute of Technology
8:35 AM	Characterizing Microwave Efficiency in DNP Instrumentation by Frequency Swept EPR. Anne M. Carroll, Yale University
8:55 AM	Cavity-free 9.4 Tesla EPR Spectrometer for Large Samples used in DNP Experiments. Jean-Philippe Ansermet, Ecole Polytechnique Fédérale de Lausanne
9:25 AM	Magic Angle Spinning Spheres, Electron Decoupling with CPMAS below 6 K, and DNP within Human Cells Using Fluorescent Polarizing Agents. Alexander B. Barnes, Washington University in St. Louis
9:45 AM	<i>Break</i>
Session XII: Integrated Magnetic Resonance II. (Joint Session - EPR & SSNMR) Sophia Hayes & Gail Fanucci, Chairs	
10:15 AM	Novel Aspects of Polarization Propagation and Biomolecular Applications of MAS DNP. Björn Corzilius, Goethe University
10:45 AM	Truncated Cross Effect Dynamic Nuclear Polarization: Overhauser Effect Doppelgänger. Asif Equbal, University of California Santa Barbara
11:05 AM	Breaking Concentration Sensitivity Barrier by Larger Volumes: Photonic Band-Gap Resonators for mm-Wave EPR and DNP of Microliter-Volume Samples. Alex I. Smirnov, North Carolina State University
11:35 AM	Optical Room Temperature ¹³C Hyperpolarization in Powdered Diamond. Ashok Ajoy, University of California Berkeley
12:00 PM	<i>Lunch (included with registration)</i>
Session XIII: Methods I. Dane McCamey, Chair	
1:30 PM	Pulsed Magnetic Resonance with a Free-Electron Laser. Mark Sherwin, University of California Santa Barbara
2:00 PM	Pulsed and 'in-situ' EPR at 395 GHz. Johan van Tol, National High Magnetic Field Laboratory
2:15 PM	Development of a High Field Nanoscale EPR System using NV Centers in Diamond. Benjamin Fortman, University of Southern California
2:30 PM	Automated DEER Data Processing using Bayesian Inference. Thomas H. Edwards, University of Washington
2:45 PM	Accurate and Direct Determination of Distance Distributions for Pulsed Dipolar ESR by Singular Value Decomposition. Madhur Srivastava, Cornell University
3:00 PM	<i>Break</i>
Session XIV: Methods II. Susumu Takahashi, Chair	
3:40 PM	Electron Spin Resonance with Quantum Microwaves. Audrey Bienfait, Institute of Molecular Engineering
4:10 PM	Signal Enhancement by Constructive Combination of Transmission and Reflection ESR signals using Non-Resonant Transmission Line Probe Detection. Pragya R. Shrestha, National Institute of Standards and Technology
4:25 PM	Multi-Frequency Pulsed EPR and DEER Using Rapidly Tunable Superconducting Microresonators. Abraham T. Asfaw, Princeton University
4:40 PM	Effect of Multiphoton Transitions on Detection of Long Electron Spin Relaxation Times by Double Modulation ESR Spectroscopy. Boris Rakvin, Rudjer Boskovic Institute
4:55 PM	Multi-Extreme THz ESR: Development of Mechanically Detected ESR up to the THz Region. Hitoshi Ohta, Kobe University
General Business Meeting/SharedEPR Presentation	
5:15 PM	Stefan Stoll, Chair
7:00-9:00 PM	<i>Conference Banquet & Awards Ceremony (Enjoy an evening of comradeship, fine food and recognition of peers. Pre-registration required.)</i>
8:00 PM	Welcoming Remarks. Kurt Zilm, Conference Chair
8:05 PM	A Half Century of RF, μw's and the Magic Angle. Robert G. Griffin, Massachusetts Institute of Technology
8:35 PM	EPR Awards
8:45 PM	SSNMR Awards

THURSDAY, JULY 26, 2018

Session XV: EPR Imaging / In-Vivo. Boris Epel, Chair	
8:15 AM	Redox, Oximetric and Vascular Imaging Provide Insight into the Tumor Microenvironment. Martyna Elas, Jagiellonian University
8:45 AM	Pre-clinical EPR Imaging System at 800 MHz. Mark Tseytlin, West Virginia University
9:15 AM	Molecular Oxygen: Extent of Variability in Time and Location in Preclinical Tumors. Howard J. Halpern, University of Chicago
9:30 AM	Design, Synthesis and Characterization of New Triarylmethyl (TAM) Radicals for Biomedical EPR Applications. Benoit Driesschaert, West Virginia University
9:45 AM	<i>Break</i>
Session XVI: Methods III. Stefan Stoll, Chair	
10:25 AM	The CHEESY Renaissance of Fourier-transform Detected Hole Burning in EPR. Gunnar Jeschke, ETH Zürich
10:55 AM	Development of ELDOR-detected NMR Spectroscopy at 115/230 GHz. Zaili Peng, University of Southern California
11:10 AM	²H-Cross-polarization Edited ENDOR at 94 GHz to Study the Conformation of Protein Radical Intermediates. Isabel Bejenke, Max Planck Institute for Biophysical Chemistry
11:25 AM	Exploring Frequency-swept Excitation for Distance Measurements of Spin $S = \frac{1}{2}$ Systems. Frauke Breitgoff, ETH Zürich
11:40 AM	DEER Updates are Available: Upgraded Sensitivity after RELOAD and Unmodulated Background Suppressed with the ROOPh. Sergey Milikisiyants, North Carolina State University
11:55 AM	Closing Remarks. Stefan Stoll, EPR Symposium Chair
Post-Conference Activities	
1:30 PM	SharedEPR Workshop: Software Tools for EPR Spectroscopy – Capabilities and Demonstrations

FRIDAY, JULY 27, 2018

Post-Conference Activities	
8:30 AM	SharedEPR Workshop: Software Tools for EPR Spectroscopy – Capabilities and Demonstrations