



**43rd INTERNATIONAL EPR SYMPOSIUM
JULY 25-29, 2022
COPPER MOUNTAIN, COLORADO, USA**

EPR SYMPOSIUM COMMITTEE

Fraser MacMillan (Chair)
Dane McCamey (Co-Chair 2022, Chair 2023)
Aharon Blank
Ania Bleszynski-Jayich
Christoph Boehme
Gail Fanucci
Songi Han
Stephen Hill
John McCracken
Chandrasekhar Ramanathan

AGENDA

MONDAY, JULY 25, 2022

Pre-Conference Activities	
3:00 PM - 5:00 PM	Workshop: Spin Resonance Spectroscopy at the Quantum Limit. Jarryd Pla, University of New South Wales Sydney
6:30 PM - 10:00 PM	Bruker EPR Users' Meeting & Reception

8:10 AM	Welcoming Remarks. Fraser MacMillan, EPR Symposium Chair
Methods I. Stephen Hill, Chair	
8:15 AM	Probing Spin Dynamics using EPR-on-a-chip: Methods Old and New. Michal Kern, Universität Stuttgart
8:45 AM	Practical Applications of an EPR on a Chip Device. Joseph E. McPeak, Helmholtz-Zentrum Berlin
9:00 AM	Development of an Injectable EPR Imaging Agent for Clinical Use. Joshua R. Biller, TDA Research Inc.
9:15 AM	Non-resonant Broadband ESR Sensor for Portable Retrospective Dosimetry. Pragya R. Shrestha, Theiss Research and National Institute of Standards and Technology
9:30 AM	EPR to Go. Michele Segantini, Helmholtz-Zentrum Berlin
9:45 AM	Automated Digital Tuning, Coupling and Data Acquisition for Rapid Scan EPR. Ryan C. O'Connell, West Virginia University
10:00 AM	<i>Break</i>
Methods II. Stephen Hill, Chair	
10:30 AM	Quantum Sensing: Probing Biological Systems in a New Light. Peter Maurer, University of Chicago
11:00 AM	Paving New Paths for Dipolar EPR Spectroscopy. Luis Fábregas-Ibáñez, ETH Zürich
11:15 AM	Optimizations for Frequency-swept Excitation Pulses in EPR. Paul Trenkler, Goethe University Frankfurt
11:30 AM	Proteins Under Nanoscale Spatial Confinement: What can EPR Tell Us?. Zhongyu Yang, North Dakota State University
11:45 AM	Hyperfine Decoupling of Magnetic Resonance Spectra Using Wavelet Transform. Madhur Srivastava, Cornell University
12:00 PM	<i>Lunch (included with registration)</i>
Biological I. Fraser MacMillan, Chair	
1:15 PM	Protein Structural Flexibility Viewed by SDSL-EPR Spectroscopy: From in vitro to in cell Studies. Valérie Belle, CNRS AMU
1:45 PM	Ultra-fast Bio-orthogonal Spin-labeling and DEER Spectroscopy for Measuring Protein Conformational Distributions in Mammalian Cells. Eric G. B. Evans, University of Washington
2:00 PM	Comparing the Conformational Dynamics of dsRNA and dsDNA using Orientation-selective PELDOR. Maximilian Gauger, Goethe University Frankfurt
2:15 PM	Hydrophilic TAM-based Spin Label for In-Cell Distance Measurements and Orthogonal Labeling Schemes at High Temperature. Zikri Hasanbasri, University of Pittsburgh
2:30 PM	Elucidation of Site-Specific Dynamics in Proteins from Cu(II) EPR Lineshape Analysis. Kevin Singewald, University of Pittsburgh
2:45 PM	<i>Break</i>
Biological II. Songi Han, Chair	
3:15 PM	New Triarylmethyl Radical Spin Probes and Labels for Biomedical EPR Applications. Benoit Driesschaert, West Virginia University
3:45 PM	Spectroscopic Investigation of Oxygen Tolerant [FeFe] Hydrogenases. A. Silakov, Pennsylvania State University
4:00 PM	5-Hydroxytryptophan as a Probe for Long Range Electron Transfer in Oxalate Decarboxylase. Alexander Angerhofer, University of Florida
4:15 PM	Triggered Functional Dynamics of AsLOV2 by Time-resolved Electron Paramagnetic Resonance at High Magnetic Fields. Shiny Maity, UC Santa Barbara
4:30 PM	Quantum Sensing of Light-Induced Electron Transfer in Natural Photosynthesis: A Time-Resolved 130 GHz EPR and ENDOR Study. Oleg Poluektov, Argonne National Laboratory
4:45 PM	From Method Development to Application: Combining Deuteration with Cu(II) Labels to Establish Structural Links in a Metalloregulator's Transcription Cycle. Joshua Casto, University of Pittsburgh
5:30-7:00 PM	<i>Conference Reception (included with registration)</i>
Posters	
7:00-9:00 PM	Authors Present for Posters Labeled A

Materials I. Christoph Boehme, Chair	
8:15 AM	On the Magnetic Properties of Photogenerated Organic Three-spin Systems. Sabine Richert, University of Freiburg
8:45 AM	Exciton Dynamics on Triplet-Triplet Annihilation Upconversion in Organic Semiconductors Revealed by Time-Resolved EPR. Tsubasa Okamoto, Kobe University
9:00 AM	Magnetic Edges and Electron Coherence in Molecular Graphene Nanoribbons using Porphyrins as Spin Injectors. Michael Slota, University of Oxford
9:15 AM	Spin Relaxation Dynamics in Radical-Pair Processes at Low Magnetic Fields. Taniya H. Tannahewa, University of Utah
9:30 AM	<i>Break</i>
Methods III. Songi Han, Chair	
10:15 AM	Shining a Light on Electron Spin Resonance: Light-induced Pulsed Dipolar Spectroscopy. Alice M. Bowen, University of Manchester
10:45 AM	Singlet Fission and Spin Dynamics in Novel Bipentacene Complexes: Time-Resolved EPR Study. Jens Niklas, Argonne National Laboratory
11:00 AM	Development of a Small Scale, Interferometric Microwave Conductivity Tool to Probe Dynamics of Photogenerated Charge Carriers. Jasleen K. Bindra, National Institute of Standards and Technology and University of Maryland
11:15 AM	Pulsed EPR Study of Vanadyl-Porphyrin Functionalized Graphene Nanoribbons. Fanmiao Kong, University of Oxford
11:30 AM	Probing the Influence of Spin-orbit Coupling on Charge Carrier Spin States in π-conjugated Polymers, Caused by Heavy Elements of Hole Injectors Based on MoO_3. Sanaz Hosseinzadeh, University of Utah
12:00 PM	<i>Lunch (included with registration)</i>
Spin Devices I. Dane McCamey, Chair	
1:15 PM	High-Field EPR Investigation of a Potential Molecular Two-Qubit Gate Based on a Cobalt Dimer. Daphné Lubert-Perquel, National High Magnetic Field Laboratory
1:45 PM	Design, Synthesis, and Coherence of Spectrally-Addressable Multiqubit Metal Complexes. Stephen von Kugelgen, Massachusetts Institute of Technology
2:00 PM	Modelling Conformational Flexibility in a Spectrally Addressable Multi-Spin Molecular Qubit Model System. Ciarán J. Rogers, University of Manchester
2:15 PM	Electron Spin-Echo Envelope Modulation at Spin Clock Transitions. Stephen Hill, National High Magnetic Field Laboratory
2:30 PM	Non-Bloch-Siegert Type Drive-Field Induced Resonance Shift of Two-Photon Spin-Resonant Transitions. Sabastian I. Atwood, University of Utah
2:45 PM	<i>Break</i>
Methods IV. Chandrasekhar Ramanathan, Chair	
3:15 PM	Plasmonic Metasurface Resonators to Enhance Terahertz Magnetic Fields for High-Frequency Electron Paramagnetic Resonance. Lorenzo Tesi, University of Stuttgart
3:45 PM	Multi-Extreme THz ESR: Developments on New Detection Methods and under High-Pressure Condition. Hitoshi Ohta, Kobe University
4:00 PM	Sample Holders for Sub-THz Electron Spin Resonance Spectroscopy. Antonín Sojka, University of California Santa Barbara
4:15 PM	Open-Source Loop-Gap Resonator for X-Band EPR Spectroscopy. Timothy J. Keller, Bridge12 Technologies, Inc.
4:30 PM	Dipolar Order in Electron Spins: An EPR Signature of Thermal Mixing DNP. Asif Equbal, University of California Santa Barbara
Posters	
7:00-9:00 PM	Authors Present for Posters Labeled B

Integrated Magnetic Resonance I. (Joint Session - EPR & SSNMR) - Fraser MacMillan presiding	
IES Fellow Award Presentation	
8:10 AM	Songi Han (IES President) to R. David Britt
8:15 AM	EPR Studies of the Enzymatic Synthesis of the Organometallic H-Cluster of [FeFe] Hydrogenase. R. David Britt, University of California Davis
8:55 AM	Combining Solid-state NMR with DEER EPR to Study Structure and Dynamics of Cross-β Fibrils. Ansgar Siemer, University of Southern California
9:15 AM	From Fast Water on Surfaces to Nearly Immobile Nano-Confined Water: Exploring and Expanding the Dynamic Range of Overhauser Dynamic Nuclear Polarization. John M Franck, Syracuse University
9:30 AM	Methyl-Driven Overhauser MAS-DNP. Frédéric Perras, Ames Laboratory
9:50 AM	<i>Break</i>
Integrated Magnetic Resonance II. (Joint Session - EPR & SSNMR) - Sophia E. Hayes presiding	
10:15 AM	Up-conversion of Radio-frequency NMR Signals to Light via a Membrane Transducer. Kazuyuki Takeda, Kyoto University
10:45 AM	Spin Textures and Quantum Sensing with Optically Hyperpolarized Nuclei. Ashok Ajoy, University of California Berkeley
11:15 AM	DNP using Spherical Rotors. Lauren Price, ETH Zürich
11:35 AM	Terahertz EPR Spectroscopy Using a 36-Tesla High-Homogeneity Series-Connected Hybrid Magnet. Thierry Dubroca, National High Magnetic Field Laboratory
12:00 PM	<i>Lunch (included with registration)</i>
Biological III. Kurt Warncke, Chair	
1:15 PM	Time-resolved DEER EPR and Solid-state NMR Afford Kinetic and Structural Elucidation of Substrate Binding to Ca²⁺-ligated Calmodulin. Thomas Schmidt, National Institutes of Health
1:45 PM	Newly-Developed dHis-Cu²⁺ Force Fields Establish Cost-Efficient Protocol for DEER Measurements at Q-band. Xiaowei Bogetti, University of Pittsburgh
2:00 PM	Comparative Evaluation of Spin Label Modeling Methods for Protein Structural Studies. Maxx Tessmer, University of Washington
2:15 PM	Local Water Concentration in Lipid Bilayers by Pulsed EPR Methods. Alex I. Smirnov, North Carolina State University
2:30 PM	In situ Pulsed Dipolar Electron Spin Resonance Spectroscopy of Membrane Protein Complexes. Benesh Joseph, Goethe University
3:00 PM	<i>Break</i>
Materials III. Christoph Boehme, Chair	
3:30 PM	Revealing Redox Processes and Probing Phase Transformations in Sodium-ion Battery Cathodes using EPR and NMR Spectroscopy. E.N. Bassey, University of Cambridge
3:45 PM	Multi-Frequency and Variable Temperature EPR Reveal Charge Carrier Position in Graphite Anodes for Li-ion Batteries. T. Insinna, University of Cambridge
4:00 PM	Prolonging Room Temperature Spin-coherence in Silicon: Magic-angle Spin-pairs in a-Si:H. U. Gerstmann, Universität Paderborn
4:15 PM	Measuring Power Spectra in Diamonds with P1 and NV Centers at 2.5 GHz. Ethan Q. Williams, Dartmouth College
4:30 PM	Non-Markovian Spin-Bath Dynamics of a Single Nitrogen-Vacancy Center in Diamond. Cooper Selco, University of Southern California
4:45 PM	Modeling the Phosphorescence Dynamics of a Metal-free Dual Singlet-triplet Emitting OLED Under Magnetic Resonance. Vagharsh Mkhitarian, University of Regensburg
5:00 PM	Dangling Bond Recombination in Amorphous Silicon Studied by Multifrequency Electrically Detected Magnetic Resonance. Hans Malissa, University of Utah
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	In the Beginning.... It's all about Electronic Structure and Molecular Dynamics. Cynthia Jameson, University of Illinois at Chicago
8:35 PM	EPR Awards
8:45 PM	SSNMR Awards

FRIDAY, JULY 29, 2022

Biological IV. Kurt Warncke, Chair	
8:15 AM	Unraveling a Ligand-Induced Twist of a Homodimeric Enzyme by Pulsed Electron–Electron Double Resonance. Dinar Abdullin, University of Bonn
8:45 AM	Pulsed EPR DEER (double electron-electron resonance) Estimation of Distribution of Dipolar Interactions Between Gd³⁺ Ions with Significant Zero-field Splitting in Biradicals in a Polycrystalline Sample. Sushil K. Misra, Concordia University
9:00 AM	Utilising Thiol Chemistry for Site-Directed Spin-Labeling of the Prion Protein Using Spin Label Rx and conducting Electron Paramagnetic Resonance Distance Measurements. T.E. Assafa, University of California Santa Cruz
9:15 AM	Proline Substitutions Impact Bridge Helix Integrity of SpyCas9 as Detected by Using Site-Directed Spin Labeling. Difei Wu, University of Southern California
9:30 AM	Protonation of Model Ionizable Sidechains in Transmembrane Protein Domains. Tatyana I. Smirnova, North Carolina State University
9:45 AM	<i>Break</i>
Spin Devices II and Materials IV. Dane McCamey, Chair	
10:15 AM	Coherent Magnonics using a Molecule-based Ferrimagnet. Ezekiel Johnston-Halperin, The Ohio State University
10:45 AM	Spin Dynamics in Singlet Fission. Thomas S. C. MacDonald, UNSW Sydney
11:00 AM	Broadband ODMR Reveals Optically Sensitive Transitions of Biexcitons in a Singlet Fission Material. G. Joshi, National Renewable Energy Laboratory
11:15 AM	A Direct Monitoring Method of Titania Photocatalytic Activity by an in situ Photoreactor-EPR Setup. Mohamed A. Morsy, King Fahd University of Petroleum and Minerals
11:30 AM	Nuclear Quadrupole Resonance Spectroscopy Using a Femtotesla Diamond Magnetometer. Yaser Silani, University of New Mexico
11:45 AM	Closing Remarks. Fraser MacMillan, EPR Symposium Chair and Dane McCamey, EPR Symposium Co-chair