64th Annual
ROCKY MOUNTAIN CONFERENCE
ON MAGNETIC RESONANCE

Final Program and Abstracts

August 3-7, 2025

Snowbird Resort & Conference Center
Snowbird, Utah, USA

www.rockychem.com

64th ROCKY MOUNTAIN CONFERENCE ON MAGNETIC RESONANCE

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46th International EPR Symposium

TABLE OF CONTENTS

Organizers and Chairpersons *2*
Conference Supporters *2*
RMCMR Information *3*
- Registration
- Exhibit Schedule
- Altitude
- Conference Lunch
- Conference Reception

64th Rocky Mountain Conference-at-a-Glance *3*
Meeting Spaces *4*

Program Schedule - 46th International EPR Symposium *5*
- Monday Oral Sessions
- Tuesday Oral Sessions
- Wednesday Oral Sessions
- Thursday Oral Sessions
- EPR Poster Sessions

RMCMR Abstracts

- Oral Abstracts *11*
- Poster Abstracts *78*

Index of Presenters *106*

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ORGANIZERS AND CHAIRPERSONS

CONFERENCE CHAIR:

Kurt W. Zilm
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kurt.zilm@yale.edu

EPR SCIENTIFIC COMMITTEE:

Stephen Hill – **Chair**
Florida State University

Mrignayani Kotecha – **Vice-Chair**
Chief Executive Officer, O2M

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New York University

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University of Utah

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Northwestern University

Petr Neugebauer
Central Euro. Inst. of Tech.

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Penn State University

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University of Washington

Mark Tseytlin
West Virginia University

CONFERENCE SUPPORTERS & EXHIBITORS

ACERT

Bruker

ColdEdge Technologies

Cryogenic Ltd

FeMi Instruments, LLC

High Q Technologies

National High Magnetic Field Lab

O2M Technologies, LLC

Rotunda Scientific Technologies

ROCKY MOUNTAIN CONFERENCE INFORMATION

REGISTRATION

Admission to all technical sessions and the exhibition is by name badge only. Registration materials may be picked up between 10:00 am and 5:00 pm on Sunday, August 3 or anytime between 8:00 am and 5:00 pm Monday, August 4 through Wednesday, August 6 or 8:00 am and 11:30 am on Thursday, August 7.

EXHIBITION SCHEDULE

Monday, August 4
10:00 a.m. - 7:00 p.m.
Conference Reception - 5:30 p.m. – 7:00 p.m.
Tuesday, August 5
9:00 a.m. – 5:00 p.m.
Wednesday, August 6
9:00 a.m. – 4:00 p.m.

ALTITUDE

Snowbird is approximately 8,100 feet above sea level. The acclimatization process is inhibited by dehydration, over-exertion, alcohol and other depressant drugs. Please take the following precautions regarding high altitude:

- Take it easy; don't over-exert yourself

- Light activity during the day is better than sleeping because respiration decreases during sleep, exacerbating the symptoms.

- Avoid tobacco, alcohol and other depressant drugs including, barbiturates, tranquilizers, and sleeping pills.

- Eat a high carbohydrate diet

- Drink three to four times more water than usual.

CONFERENCE LUNCH

A complimentary lunch is being provided August 4, 5 and 6 to all registered conference attendees.
The lunch will be served in Ballroom 2 each designated day from 11:30 a.m. – 1:00 p.m.

CONFERENCE RECEPTION

Monday evening from 5:30 p.m. to 7:00 p.m., all attendees are cordially invited to join in on beverages and hors d'oeuvres. Unwind from the day's events and continue the "Rocky Mountain Conference" experience. Check out all of the latest products and services as the reception is held right in the exhibition area.

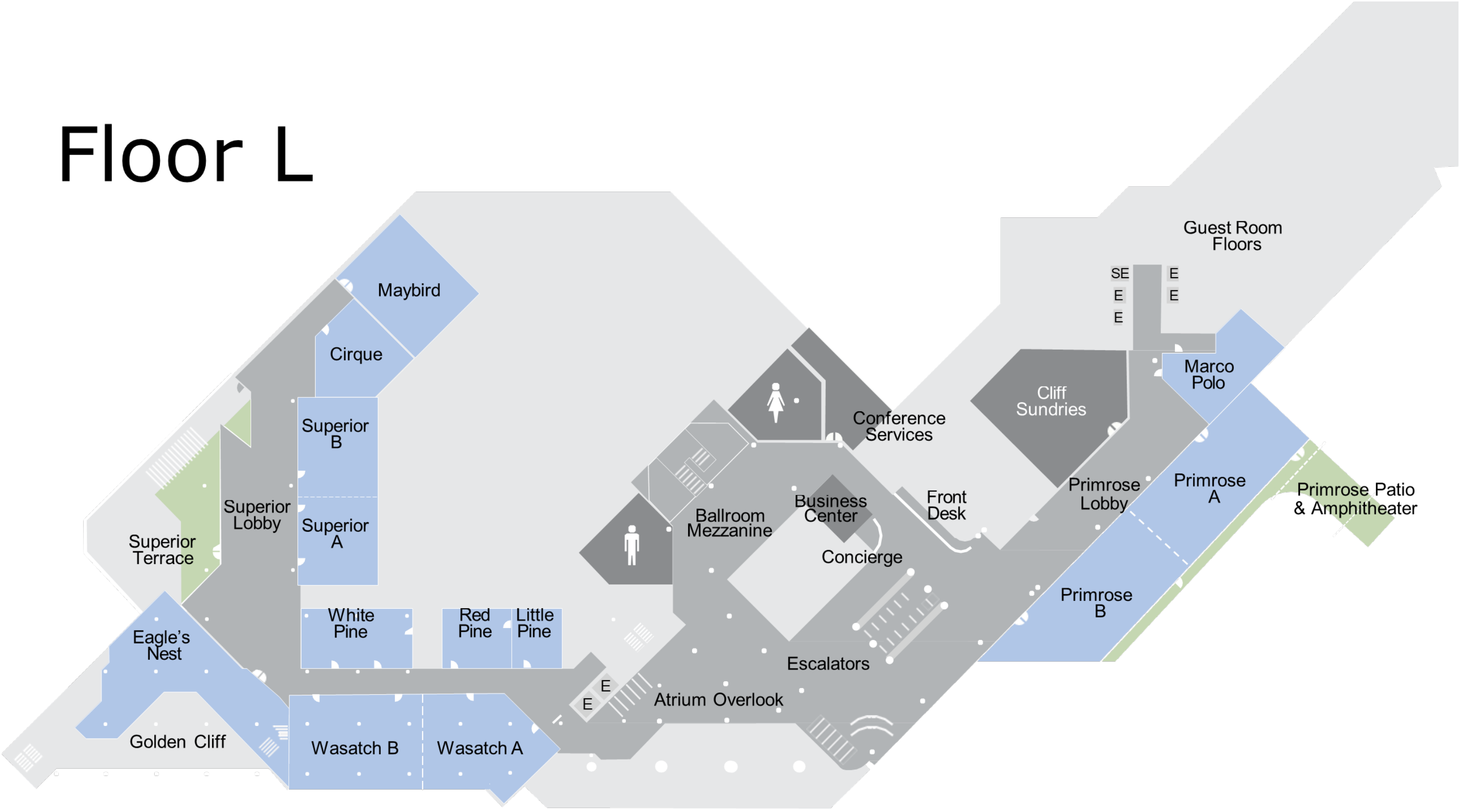
CONFERENCE-AT-A-GLANCE

Event	Location	Sunday		Monday		Tuesday		Wednesday		Thursday		Friday	
		a.m.	p.m.	a.m.	p.m.	a.m.	p.m.	a.m.	p.m.	a.m.	p.m.	a.m.	p.m.
Bruker Users Meeting	**Ballroom 2**		▨										
EPR Lectures	**Ballroom 1**			▨	▨	▨	▨	▨	▨	▨			
EPR Posters	**Superior**			▨	▨	▨	▨	▨	▨	▨			
Exhibition	**Ballroom Foyer**			▨	▨	▨	▨	▨	▨				

SNOWBIRD CONFERENCE CENTER MEETING SPACE

Floor L1

Floor L



EPR SYMPOSIUM ORAL SESSIONS AGENDA

SUNDAY, AUGUST 3, 2025

Pre-Conference Activities	
6:00 PM – 9:30 PM	**Bruker EPR Users' Meeting & Reception**

MONDAY, AUGUST 4, 2025

Imaging I		**Mrignayani Kotecha, Chair**
8:00 AM	100	**EPR Oxygen Imaging: Methodology, Instrumentation and Applications.** Boris Epel, University of Chicago
8:30 AM	101	**Advanced in EPR Imaging: Instrumentation, Algorithms and Applications.** Mark Tseytlin, West Virginia University
8:50 AM	102	**OxyTrack: a Novel Needle Sensor for *in situ* Oximetry.** Ryan O'Connell, Dartmouth College
9:10 AM	103	**EPR and Computational Study on the Radiation-induced Transformations in the Nuclear Fuel Cycle.** Ilya Sosulin, University of Notre Dame, Radiation Laboratory
9:30 AM		*Break*
Methods I		**Stephen Hill, Chair**
10:00 AM	104	**Continuous-flow Electron Spin Resonance Microfluidics Device with Sub-nanoliter Sample Volume.** Aharon Blank, Technion - Israel Institute of Technology
10:30 AM	105	**Time-resolved Distance Distributions after 450 nm Excitation of a Photoresponsive Protein Domain at Room Temperature in Solution.** Mark Sherwin, University of California at Santa Barbara
10:50 AM	106	**DEER Spectroscopy With Swept Observer Pulses.** Eric R. Lowe, University of Maryland, Baltimore County
11:10 AM	107	**High-Power 263 GHz Pulsed-EPR Spectrometer for the Elucidation of Transition Metals in Protein Systems.** Zikri Hasanbasri, University of California - Davis
11:30 AM		*Lunch (included with registration)*
Radical Pairs I		**Christoph Boehme, Chair**
1:00 PM	108	**Photoinduced Polarons on Donor and Acceptor Molecules for Organic Photovoltaics Studied by Multifrequency Pulse EPR.** Claudia Tait, University of Oxford
1:30 PM	109	**EPR Study of Charge Transfer Co-crystals Structure/Function Relationship.** Raanan Carmielli, Weizmann Institute of Science
1:50 PM	110	**Spin Dynamics of SCRPs in ZnO Quantum Dot – Organic Molecule Conjugates.** Mandefro Teferi, Argonne National Laboratory
2:10 PM	111	**Spin Dynamics in Singlet Fission Oligomers and Polymers with Tetracene Pendants.** Jens Niklas, Argonne National Laboratory
2:30 PM	112	**Organic Molecules as Spin-optical Interfaces: From Magnetic Sensing to Photoredox Catalysis.** Joel Yuen-Zhou, UC San Diego
3:00 PM		*Break*
Organic Spins		**Tatyana Smirnova, Chair**
3:30 PM	113	**Heisenberg and Dipolar Spin Exchange Among Paramagnetic Probes in a Percolation Network.** David E. Budil, Northeastern University
3:50 PM	114	**EPR Spectroscopy of Chiral Polyacetylene Thin Films.** Prashanna Poudel, University of Utah
4:10 PM	115	**Insights into Triplet Vinylidenes: Electronic Structure and Stability Using Imidazopyridine Scaffolds.** Sergius Boschmann, TU Dortmund University

4:30 PM	116	**Probing the Electrical Properties of Twisted Tetrathiafulvalene Thin-Films Using cwEPR.** Matthew Ross, New York University
5:30-7:00 PM	Conference Reception (included with registration)	
Posters		
7:00-9:00 PM	Authors Present for Posters Labeled A	

TUESDAY, AUGUST 5, 2025

Spin Relaxation		**Hans van Tol, Chair**
8:00 AM	**117**	**Electron Spin Relaxation and Pulse Turning Angles of Lanthanide Complexes.** Gareth R. Eaton, University of Denver
8:30 AM	**118**	**What Governs Spin Decoherence in Condensed Matter?** Toshikazu Nakamura, Institute for Molecular Science
8:50 AM	**119**	**EPR Characterization of Molten Salt Synthesized Erbium(III) Doped Yttria Nanoparticles.** William Bittner, University of Washington
9:10 AM	**120**	**Manipulation of Spins in Pulse EPR.** Michael K. Bowman, University of Alabama
9:30 AM		*Break*
Biomolecules		**Alexey Silakov, Chair**
10:00 AM	**121**	**Structure and Dynamics of Monoclonal Antibodies using Spins, Scattering, and Simulations.** Veronika A. Szalai, National Institute of Standards & Technology
10:30 AM	**122**	**Nanotemplate Approach to Stabilize Macroscopically Aligned Lipid Bilayers and Membranes Proteins under a Broad Range of Temperatures and Hydration Levels.** Alex I. Smirnov, North Carolina State University
10:50 AM	**123**	**Structural Identification of the Building Blocks of a Small Heterogenous Amyloid Oligomer by ESR.** Tufa E. Assafa, Cornell University
11:10 AM	**124**	**Tuning Sidechain Protonation at the Membrane Interface: Implications for T-Cell Receptor Assembly.** Tatyana I. Smirnova, North Carolina State University
11:30 AM		*Lunch (included with registration)*
Spin Labeling		**Peter Qin, Chair**
1:00 PM	**125**	**Development of EPR Technologies to Elucidate Signaling Selectivity in GPCRs.** Michael T. Lerch, Medical College of Wisconsin
1:30 PM	**126**	**In-cell Cu(II)-NTA Labeling for EPR Distance Measurements.** Hannah Hunter, University of Pittsburgh
1:50 PM	**127**	**Rigid Cu(II) Spin Label Sensitive to DNA Conformational Flexibility in Protein-DNA Complexes.** Shramana Palit, University of Pittsburgh
2:10 PM	**128**	**Photochemical and Mechanical Activation of Metal Oxide Additives Drives Radical Formation in Lubricating Oils: an EPR Spin-Trapping Study.** Julie Matheny, North Carolina State University
2:30 PM	**129**	**Flavoproteins as Native and Genetically Encoded Spin Probes for in Cell ESR Spectroscopy.** Timothée Chauviré, Cornell University
3:00 PM		*Break*
Metals		**Veronika Szalai, Chair**
3:30 PM	**130**	**EPR and FIRMS Characterization of the Magnetic Anisotropy in a Set of Metalorganic $Mn^{III}[R\text{-}sal_{2}323]^{+}$ Spin-Crossover Complexes.** Brittany Grimm, NHMFL
3:50 PM	**131**	**Electronic Wavefunction Delocalization Beyond the Metallic Core of Palladium Dodecanethiolate Nanoparticles: Revealed through Pulse ESR.** Kristen M. Aviles, Pennsylvania State University

4:10 PM	**132**	**Lessons from Preclinical EPR pO2 Oxygen Images.** Howard Halpern, University of Chicago
4:30 PM	**133**	**ACERT: A Service Resource for ESR Researchers.** Jack H. Freed, Cornell University
Posters		
7:00-9:00 PM		Authors Present for Posters Labeled B

WEDNESDAY, AUGUST 6, 2025

Color Centers	**Claudia Avalos, Chair**	
8:00 AM	**134**	**Shallow Donors in Hexagonal Silicon Carbide: A Qubit Candidate Investigated by Pulsed EPR and Pulsed ENDOR at High Field.** Johan van Tol, Florida State University
8:30 AM	**135**	**Optical Detection of Carbon-13 NMR in Diamond for Rotation Sensing.** Maxwell D. Aiello, University of New Mexico
8:50 AM	**136**	**Optically Detected Coherent Spin Control of Organic Molecular Color Center Qubits.** Sebastian M. Kopp, Northwestern University
9:10 AM	**137**	**Anisotropies of Electrically Detected Multiphoton EPR Transitions in the Nonperturbative Resonant Drive Regime.** Chanhyun Pak, University of Utah
9:30 AM		*Break*
Methods II		**Mark Sherwin, Chair**
10:00 AM	**138**	**Dielectric Resonator Optimization for EPR Spectroscopy and Solid-state MASERs.** Christopher W. M. Kay, Saarland University
10:30 AM	**139**	**A Free-electron-laser-powered Agile Pulsed Electron Spin Resonance (FEL AESR) Spectrometer.** Alex Giovannone, University of California, Santa Barbara
10:50 AM	**140**	**Multi-Extreme THz ESR: Past and Future.** Hitoshi Ohta, Kobe University
11:10 AM	**141**	**Non-Uniform Sampling for Pulsed Dipolar Electron Spin Resonance Spectroscopy.** Nimesh Srivastava, EZ Diagnostics Inc.
11:30 AM		*Lunch (included with registration)*
DEER/PELDOR		**Christopher Kay, Chair**
1:00 PM	**142**	**Following Conformational Changes in LbuCas13a from Apo to the Ternary Complex with PELDOR.** Olav Schiemann, University of Bonn
1:30 PM	**143**	**Breaking the Cycle: How Enzymes Control Oxygen Rebound for Versatile Biocatalysis.** Alexey Silakov, Pennsylvania State University
1:50 PM	**144**	**Complete Expressions for Accurate Simulations of Strong and Weak-Pulse DQC and DEER Experiments.** Aritro Sinha Roy, Cornell University
2:10 PM	**145**	**Q-band Double Quantum Coherence ESR for Sensitive Nitroxide-based Distance Measurements.** Alysia Mandato, University of Pittsburgh
2:30 PM	**146**	**Structural Integrity and Side-Chain Interaction at the Loop Region of the Bridge Helix Modulate Cas9 Substrate Discrimination.** Peter Z Qin, University of Southern California
3:00 PM		*Break*
Imaging II		**Mark Tseytlin, Chair**

3:30 PM	147	**50 Years of EPR Oximetry from Capillary to Clinic.** Periannan Kuppusamy, Dartmouth College
4:00 PM	148	**Tumor Tissue EPR Oxygen Imaging for Optimizing Interstitial Photodynamic Therapy.** Mrignayani Kotecha, O2M Technologies, LLC
4:20 PM	149	**L-band EPR Spectrometer and Resonators for Rapid Scan.** Tanden A. Hovey, University of Denver
4:40 PM	150	**Trityl OXO71 Distribution Following Intravenous Injection in Rhesus Macaques.** Christopher D. Kroenke, Oregon Health & Science University
7:00-9:00 PM	**Conference Banquet & Awards Ceremony**	
(Enjoy an evening of comradeship, fine food and recognition of peers. Pre-registration required.) - Speaker John McCracken		

THURSDAY, AUGUST 7, 2025

Hyperploarization		**Alex Smirnov, Chair**
8:00 AM	151	**Liquid-State DNP at 263 GHz: Advanced Instrumentation to Boost High-Resolution NMR Spectroscopy.** Igor Tkach, Max Planck Institute for Multidisciplinary Sciences
8:30 AM	152	**Pump-induced Dipolar Order to Evaluate Electron Spin Connectivity and Many-body Effects.** Joshua S. Straub, Northwestern University
8:50 AM	153	**Coherent Control Over Nuclear Hyperpolarization for Storage Using an Optically Initializable Chromophore-radical System.** Hoang Le, Northwestern University
9:10 AM	154	**Detecting the Effects of Chirality-Induced Spin Selectivity on Electron Donor–Acceptor Molecules.** Matthew D. Krzyaniak, Northwestern University
9:30 AM		*Break*
Radical Pairs II		**Claudia Tate, Chair**
10:00 AM	155	**Photogenerated Spin-Correlated Radical Pairs in Biological, Organic, and Organic-Inorganic Donor-Acceptor Systems.** Oleg G. Poluektov, Argonne National Laboratory
10:30 AM	156	**Observation of Multi-mode Spin-Rabi Oscillation of Strongly EPR Driven Polaron Pairs In a Pi-Conjugated Polymer.** Bonaventure A. Odeke, University of Utah
10:50 AM	157	**Quintet-to-Radical Spin Polarization Transfer in Pentacene–Radical Hybrid Polymers.** Jasleen Bindra, Argonne National Laboratory
11:10 AM	158	**Structural Contributions to Spin-Exchange Interactions and Spin Polarization in Pentacene-Radical Dyads.** Claudia E. Avalos, New York University

64TH ROCKY MOUNTAIN CONFERENCE ON MAGNETIC RESONANCE

46TH INTERNATIONAL EPR SYMPOSIUM POSTER SESSIONS AGENDA

MONDAY, AUGUST 4 • 7:00–9:00 p.m. *(Authors Present for Posters Labeled A)*

TUESDAY, AUGUST 5 • 7:00–9:00 p.m. *(Authors Present for Posters Labeled B)*

A	200	**Broadband and Selective Inversion of Electron Spins at Q-band Frequencies.** Dmitry Akhmetzyanov, Bruker BioSpin Corp.
B	201	**Development of Rapid-Scan EPR Spectrometer and Imager at L-band (1.0 GHz).** Georgina Amassah, University of Denver
A	202	**Multifrequency Study of Multiphoton Electron Paramagnetic Resonances in Crystalline Gd^{3+}:YVO_4.** Sabastian Atwood, National High Magnetic Field Laboratory
B	203	**Electronic Wavefunction Delocalization Beyond the Metallic Core of Palladium Dodecanethiolate Nanoparticles: Revealed through Pulse ESR**. Kristen Aviles, Pennsylvania State University
A	204	**Optomechanical Phase Shifters for Free-electron-laser Powered Agile Pulsed Electron Spin Resonance Spectroscopy.** Casey Bernd, University of Santa Barbara
B	205	**Quintet-to-Radical Spin Polarization Transfer in Pentacene–Radical Hybrid Polymers.** Jasleen Bindra, Argonne National Laboratory
A	206	**EPR Characterization of Molten Salt Synthesized Erbium(III) Doped Yttria Nanoparticles.** William Bittner, University of Washington
B	207	**An EDMR and NZFMR Study of Defects Generated in SiO_2 by High Electric Field Gate Stress.** George Bodenschatz, Pennsylvania State University
A	208	**Near Zero Field Magnetoresistance and Electrically Detected Magnetic Resonance Investigation of 4H-SiC PN Junctions.** Kaila Burgess, Penn State University
B	209	**Flavoproteins as Native and Genetically Encoded Spin Probes for in Cell ESR Spectroscopy.** Timothee Chauvire, Cornell University
A	210	**Measurement of TEMPO Reduction to Determine Storage Effects on Antioxidant Levels in Fruits and Vegetables II.** Emily Cheng, Steppingstone MAgnetic Resonance Training Center
B	211	**Probing Alternating Exchange Interactions in a Molecular Spin Chain via HFEPR.** Luan de Lima, Brno University of Technology (CEITEC - BUT)
A	212	**Advances in Distance Measurement Throughput and Sensitivity through a Superconducting Resonator Platform.** Austin Gamble Jarvi, High Q Technologies
B	213	**High-Power 263 GHz Pulsed-EPR Spectrometer for the Elucidation of Transition Metals in Protein Systems.** Zikri Hasanbasri, University of California - Davis
A	214	**Antioxidant Loaded Beta-Cyclodextrin Nanofibers for Preventing Edible Oil Degradation.** Mariam Hasany, Cornell University
B	215	**In-cell Cu(II)-NTA Labeling for EPR Distance Measurements.** Hannah Hunter, University of Pittsburg
A	216	**Optically Detected Magnetic Resonance Spectroscopy of Carbon and Nitrogen in Soil and Plant Analytes Using a Microfluidic Diamond Quantum Sensing Platform.** Sehrish Iqbal, University of Nebraska Lincoln
B	217	**Development of Hardware and Protocols for Ex-Vivo Rat Liver Oxygen Imaging.** Mrignayani Kotecha, O2M Technologies, LLC
A	218	**Coherent Control Over Nuclear Hyperpolarization for Storage Using an Optically Initializable Chromophore-radical System.** Hoang Le, Northwestern University
B	219	**Two-Axis Rotating Sample Holder for Cryogenic, High Field EPR.** Wei-Hsu (Wish) Lin, University of California, Santa Barbara

A	220	**Probing Fundamental Magneto-Structural Properties of Vanadyl Porphyrins as Molecular Spin Qubits.** Molly Lockart, Samford University
B	221	**Q-band Double Quantum Coherence ESR for Sensitive Nitroxide-based Distance.** Alysia Mandato, University of Pittsburg
A	222	**Towards Quantum Diamond Microscope for Real-space, Wide-field Hyperpolarized NMR Imaging.** Camille McDonnell, University of Maryland, College Park
B	223	**Photogenerated Spin-Correlated Radical Pairs in Silicon Quantum Dot– Organic Molecule Conjugates.** Seyedeh Shadi Mir Mohammadi, University of Utah
A	224	**Detection of Multiple Components in Closely Spaced DEER Distance Distributions via Continuous Wavelet Transform.** Utkarsh Misra, Cornell University
B	225	**Electrostatics of the Membrane Interface Revealed by EPR of Lipid-Based pH-Sensitive Probes.** Ngan Nguyen, North Carolina State University
A	226	**OxyTrack: a Novel Needle Sensor for *in situ* Oximetry.** Ryan O'Connell, Dartmouth College
B	227	**Observation of Multi-mode Spin-Rabi Oscillation of Strongly EPR Driven Polaron Pairs In a Pi-Conjugated Polymer.** Bonaventure Odeke, University of Utah
A	228	**Rigid Cu(II) Spin Label Sensitive to DNA Conformational Flexibility in Protein-DNA Complexes.** Shramana Palit, University of Pittsburgh
B	229	**Probing the Electrical Properties of Twisted Tetrathiafulvalene Thin-Films Using cwEPR .** Matthew Ross, New York University
A	230	**Enabling Enhanced Time-Resolved High-Field EPR of Protein Dynamics with a Quasioptical Sample Holder.** Johanna Schubert, University of California, Santa Barbara
B	231	**High Frequency NMR Spectroscopy With NV Centers in Diamond.** Janis Smits, University of New Mexico
A	232	**EPR and Computational Study on the Radiation-induced Transformations in the Nuclear Fuel Cycle.** Ilya Sosulin, University of Notre Dame, Radiation Laboratory
B	233	**Benchmarking Density Functional Theory for the Prediction of Fluoroalkyl Radical EPR Signatures.** Isaac Spackman, Colorado School of Mines
A	234	**A Comprehensive Set of Distance Rulers for Pulse Dipolar ESR Spectroscopy.** Madhur Srivastava, Cornell University
B	235	**Magnetic Resonance Spectroscopy of a Model Hydrogenase.** Pathorn Teptarakulkarn, University of California Los Angeles
A	236	**High-field EPR Analysis of Co- and Fe-based Metal Complexes: Unraveling Electronic and Geometric Properties.** Kavipriya Thangavel, National High Magnetic Field Laboratory
B	237	**Time-resolved Electron Paramagnetic Resonance for Silicon Quantum Dots with Radical Organic Ligands.** Alexander Yount, University of Utah

100 EPR Oxygen Imaging: Methodology, Instrumentation and Applications.

Boris Epel

Center for EPR Imaging in Vivo Physiology, University of Chicago, IL 60615
O2M Technologies, Chicago, IL 60612

Electron Paramagnetic Resonance (EPR) oxygen imaging is a non-invasive technique that enables spatial mapping of oxygen concentration within biological tissues. It relies on the paramagnetism of molecular oxygen, which affects the relaxation of spin probes introduced into the system. The unique property of EPR imaging is the ability to accurately map oxygen concentrations with high sensitivity and spatial resolution. EPR oxygen imaging offers a direct, quantitative, and real-time assessment of oxygen levels without relying on indirect metabolic markers. This method is valuable in studying tumor hypoxia, cancer treatment targeting, and therapy response evaluation. New application areas extend to organ preservation and bioengineering.

The presentation will cover innovations in EPR instrumentation and soluble probes imaging methodology including digital data processing as well as recent applications of this technology for cancer research and the analysis of spin probe pharmacokinetics and its effects on the observed oxygen in live animals.

ORAL SESSION

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101 Advanced in EPR Imaging: Instrumentation, Algorithms and Applications.

Mark Tseytlin[1,2,3], Oxana Tseytlin,[1,3]

[1] West Virginia University, School of Medicine, Dept Biochemistry, 64 Medical center Dr, HSC-N, Morgantown, WV, 26506, USA;

[2] WVU Cancer Institute, 1 Medical Center Dr, Morgantown, WV, 26506, USA;

[3] West Virginia University, In vivo Multifunctional Magnetic Resonance center, 64 Medical center Dr, HSC-S, Morgantown, WV, 26506, USA.

Recent advances in rapid scan (RS) EPR imaging will be presented, including the development of a 30 cm-bore magnet RS-EPR system with locally designed and fabricated “fingerprint” gradient coils, automatic frequency tuning and coupling, and integrated control software. We also report a novel 4D image-reconstruction algorithm optimized for rapid, high-resolution processing of large datasets and fast data conversion. This algorithm overcomes computational limits in both time and resources and enables 5D spatial–spectral–temporal imaging that demands extensive computation. In vivo and bioprinting applications will be demonstrated, with a focus on cancer imaging and bioprinting [1].

1. Sarvari S, McGee D, O'Connell R, Tseytlin O, Bobko AA, Tseytlin M. Electron Spin Resonance Probe Incorporation into Bioinks Permits Longitudinal Oxygen Imaging of Bioprinted Constructs. Mol Imaging Biol. 2024 Jun;26(3):511-524

ORAL SESSION

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102 OxyTrack: a Novel Needle Sensor for *in situ* Oximetry.

Ryan C O'Connell,[1] Maciej Kmiec,[1] Sergey V Petryakov,[1] Conner S Ubert,[1,2] Marthony L Robins,[1,2] Eugene Demidenko,[3] Philip E Schaner,[1,4] Aharon Blank,[5] Periannan Kuppusamy[1,2,4]

[1]Department of Radiology, Geisel School of Medicine, Dartmouth College, Hanover, NH, USA

[2]Thayer School of Engineering, Dartmouth College, Hanover, NH, USA

[3]Department of Biomedical Data Science, Dartmouth College, Hanover, NH, USA

[4]Department of Radiation Oncology and Applied Sciences, Geisel School of Medicine and Dartmouth-Hitchcock Hospital, Lebanon, NH, USA

[5]Schulich Faculty of Chemistry, Technion, Israel, Institute of Technology, Haifa, Israel

A novel device for in situ oximetry, called OxyTrack, has been developed using OxyChip as the EPR oxygen-sensitive reporter. OxyTrack is a coax-tip resonator with an asymmetrical shunt between a grounded needle and an internal transmission line. The length of the transmission line between the needle tip and coupling capacitor determines the resonance frequency. The design has been tested with 300MHz pulse EPR as well as L-band and X-band CW EPR using the same resonator. Several OxyTrack designs have been constructed with needle outer diameter between 0.5–1 mm and needle length 3–17 cm and utilizing brass, nickel silver, or titanium outer needles. The following experiments were all conducted with a CW L-band instrument. The oxygen calibration was linear with standard error of inverse prediction (SEIP) 0.32 mmHg. OxyTrack showed excellent SNR at low power; SNR values of 86 and 144 were demonstrated at incident RF power of 45 and 126 nW, respectively. No significant change in signal intensity or measured linewidth was observed after insertion at depths up to 17 cm. In contrast, a standard surface resonator could measure signal up to only 5-mm deep using the same OxyChip reporter. It was also found that OxyTrack orientation with respect to the main magnetic field B_0 did not affect signal intensity or measured linewidth. Response of the OxyTrack to sudden change in oxygen concentration (between nitrogen and air oxygenation) took 60 seconds to reach equilibrium. The OxyTrack resonator was shown to be compatible with the medical imaging modalities CT and MRI. Finally, OxyTrack was used a mouse model of cancer (SCC7) to demonstrate differential response to 100% oxygen breathing in muscle and tumor. Overall, OxyTrack is an exciting new sensor for EPR oximetry.

ORAL SESSION

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Tel: 623-297-0062, E-mail: f007kzy@dartmouth.edu

103 EPR and Computational Study on the Radiation-induced Transformations in the Nuclear Fuel Cycle.

Ilya Sosulin[1], Aliaksandra Lisouskaya[1]

[1]Radiation Laboratory, University of Notre Dame, Notre Dame, Indiana 46556

Extraction separation plays a crucial role in the nuclear fuel cycle by utilizing specific organic ligands designed to selectively recover fuel components and radioactive fission products from waste solutions. Additionally, supplementary compounds are employed to regulate process conditions, including pH and preventing third-phase formation. Among the chemical classes commonly utilized are phosphoric acid esters (e.g., tributyl phosphate [TBP], dioctyl phosphate [DOP]), phosphine oxides (e.g., octyl(phenyl)-N,N-diisobutylcarbamoylmethylphosphine oxide [CMPO]), phosphonates (e.g., dibutyl((diethylamino)carbonyl)phosphonate [DBDECP]), diglycolamides (e.g., N,N,N?,N?-tetraoctyl diglycolamide [TODGA]), N,N-dialkyl amides (e.g., N,N-bis(2-ethylhexyl)butanamide [DEHBA], di-2-ethylhexylisobutyramide [DEHiBA]), carboxylic acids (e.g., oxalic acid [OA], lactic acid [LA], citric acid [CA]), and acetohydroxamic acid (AHA).

Considering these ligands are exposed to ionizing radiation, their radiolytic stability becomes a critical factor affecting extraction efficiency and solvent longevity. In this study, we present a comprehensive investigation of radiation-induced transformations of these ligands in both organic and aqueous phases using electron paramagnetic resonance (EPR) spectroscopy and quantum chemical calculations. The radiation-chemical yield of paramagnetic species in neat TBP exposed to X-rays was quantitatively assessed using the spin trapping method, although structural insights provided by this method remain limited. To clarify radical structures formed upon irradiation, we conducted EPR studies at 77 K on electron-beam irradiated ligands. In all cases, carbon-centered radicals were identified. Subsequent thermal annealing induced conformational relaxations without further chemical transformations.

In the aqueous phase, the radiolytic fate of ligands is influenced by reactions with water radiolysis products, particularly hydroxyl radicals. Using continuous-flow EPR spectroscopy, we investigated these reactions with selected organic acids, enabling the determination of radical structures, as well as their bimolecular decay kinetics.

ORAL SESSION

Ilya S. Sosulin, University of Notre Dame, Radiation Laboratory, 105A Notre Dame Radiation Laboratory, Notre Dame, Indiana, 46556, United States

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104

Continuous-flow Electron Spin Resonance Microfluidics Device with Sub-nanoliter Sample Volume.

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Electron spin resonance (ESR) spectroscopy of small-volume samples is critical when the sample amount is limited, such as for rare biological molecules, isotopically enriched compounds, or small single crystals. To maximize absolute spin sensitivity in such cases, micro-resonators have been developed, some optimized for solids and others for liquids. An important advancement is integrating microfluidic capabilities into ESR micro-resonators, enabling convenient handling of minute liquid samples. However, existing microfluidic ESR devices generally lack support for continuous flow, which is essential for dynamic experiments such as monitoring chemical reactions or probing heterogeneity in single-cell populations. Single-cell analysis is increasingly recognized as essential in biology and medicine, offering insights into disease diagnosis, drug delivery, and cell communication. Despite its promise, single-cell ESR analysis faces major challenges, notably the need to sensitively and rapidly process extremely small, dynamic samples.

In this work, we present a new microfluidic ESR device specifically designed to address these challenges. The system combines a high-sensitivity surface microresonator (~9.5 GHz, ~50×50 μm field focus) with a 3D-printed quartz microfluidic chip, featuring a 50×25 μm channel aligned with the resonator's microwave magnetic field maximum. The design minimizes dielectric losses and is compatible with standard microfluidic connectors, enabling easy integration with manual or automated flow systems. We characterize the electromagnetic performance of the system and demonstrate its capabilities through pulsed and continuous-wave ESR measurements using trityl spin probes. Our results highlight the potential of this microfluidic ESR platform for enabling future single-cell chemical and physical analyses, providing a new tool for dynamic, high-sensitivity measurements at the individual cell level.

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ORAL SESSION

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105 Time-resolved Distance Distributions after 450 nm Excitation of a Photoresponsive Protein Domain at Room Temperature in Solution.

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Experiments in protein kinematics, which we define as *the time-evolution of the distribution of distances between pairs of residues in a protein after excitation by a trigger*, form an important frontier in biology. We have recently demonstrated field-domain rapid-scan time-resolved Gd-Gd electron paramagnetic resonance (rs-TiGGER) at 240 GHz and 8.6 T on the photoresponsive protein domain AsLOV2 after excitation with a pulse of 450 nm light at room temperature in solution.[1] The protein was labeled with spin-7/2 Gd-sTPATCN near the C terminus, which is on a J-a helix known to unfold upon light activation, and near the N-terminus. RS-TiGGER spectra were recorded at 24 kHz over 500 s. Upon laser illumination, the linewidth dropped, indicating reduced dipolar broadening associated with the J-alpha helix unfolding and increasing separation between spin labels, and then recovered exponentially. A 2D data matrix was constructed, with each column representing the average of 25,000 rs-TiGGER spectra, and each row indexed by the time at which the spectrum was recorded. Principal component analysis (PCA) yielded two time-dependent principal components, consistent with a folded and partially-unfolded state. The entire data matrix was fitted assuming that the distance distribution consisted of two Gaussians whose relative weights sum to a constant, and vary exponentially in time with a single exponential time constant. The effects of dipolar broadening were modeled by convolving rotationally-narrowed Pake patterns with spectra not broadened by dipolar coupling. We conclude that roughly 90% of proteins unfold after light activation, and refold with a time constant of 213 s at 10°C. The mean distance in the folded (unfolded) state is 3.2 nm (? 4.5 nm). The potential of rs-TiGGER for future protein kinematics experiments will be compared with that of time-resolved serial X-ray crystallography, FRET, and freeze-quenching followed by DEER, ssNMR, or cryo-EM. Supported by NSF-MCB 2025860.

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ORAL SESSION

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106 DEER Spectroscopy With Swept Observer Pulses.

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We present a novel variant of 4-puse double electron-electron resonance (DEER) spectroscopy. In general, the absolute modulation of the DEER signal produced is proportional to the numbers of both pump and observer spins excited. Using swept pump pulses has already been shown to improve the modulation depth by increasing the number of pumped spins.1 We show that it is possible to use swept observer pulses in combination with a swept pump pulse to maximize the excitation bandwidths of both pump and observer spins. The swept observer pulses are designed such that phase dispersion in the echo is avoided. The resulting DEER signal is simulated for an exemplary nitroxide spectrum at Q-band frequency and is compared with the signal produced with standard Gaussian observer pulses.2 We include the effect of the resonator transmission profile and the tradeoff between the enhanced observer bandwidth and the longer total sequence duration in the presence of dephasing.

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ORAL SESSION

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107 High-Power 263 GHz Pulsed-EPR Spectrometer for the Elucidation of Transition Metals in Protein Systems.

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Advanced Pulsed-Electron Paramagnetic Resonance (EPR) studies of transition metals in biological complexes at high frequencies demand stringent requirements. First, the sample space must be manageable for users to load in their solution with sufficient spins, which can be difficult with typical resonators at high frequencies. Second, the pulses should be sufficiently short to enable reasonable excitation of the spins, which requires significant microwave power. Here, we develop a quasi-optical[1] 263 GHz pulsed-EPR spectrometer equipped with a non-resonant cavity and a world-unique 10 W-Travelling Wave Tube (TWT) amplifier[2]. The cavity enables us to load samples up to ~10-12 uL, comparable to volumes at Q-band. Additionally, the 10 W TWT amplifier enables a pi-pulse of 60 ns. Furthermore, the TWT has a 10-GHz bandwidth, ensuring the capabilities of multi-frequency advanced pulsed techniques. Overall, the high-powered 263 GHz pulsed-EPR spectrometer opens the avenue for elucidating transition metals in various biological and medical contexts. Supported by NIH 1R35GM126961.

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ORAL SESSION

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108 Photoinduced Polarons on Donor and Acceptor Molecules for Organic Photovoltaics Studied by Multifrequency Pulse EPR.

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The conversion of solar energy to electricity in organic photovoltaics relies on the generation of charged states (polarons) on organic donor and acceptor molecules by photoinduced charge separation, followed by transport of these charges to the electrodes. Advances in organic photovoltaics are driven by the design of improved donor and acceptor molecules, and an in-depth understanding of how molecular structure and electronic properties affect device efficiency promises to unlock further progress. By exploiting the electron spin associated with each charge, EPR can provide crucial molecular-level insights, for example through the characterization of spin and charge delocalization, which are believed to play a significant role in promoting efficient charge separation and charge transport. We have characterized the EPR spectral signatures of photogenerated polarons in a series of donor:acceptor blends for organic photovoltaics using multi-frequency EPR, exploiting relaxation-filtered and EDNMR-induced EPR to disentangle overlapping spectral contributions.[1] The characterization of ^{1}H, ^{19}F and ^{14}N hyperfine couplings by ENDOR and HYSCORE combined with DFT calculations revealed varying extents of spin delocalization for polarons on donor polymers and on different classes of acceptor molecules. In order to more accurately model the ENDOR data of these systems characterized by significant intrinsic heterogeneity, our simulations of the experimental results employed a regularized least-squares fitting approach guided by DFT predictions.[2]

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ORAL SESSION

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109 EPR Study of Charge Transfer Co-crystals Structure/Function Relationship.

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Organic charge-transfer (CT) co-crystals exhibit unique electronic and magnetic properties depending on their molecular packing structures and aggregate states which exhibit a variety of novel properties through multicomponent synergistic and collective effects. Previously we presented that Anthracene/ tetracyanoquinodimethane (TCNQ) charge transfer co-crystals have a localized spin with a unique long relaxation times as a results of its mixed stack packing in the crystal.

Here we present the results of our charge transfer co-crystals screening study, which resulted with three more charge transfer co-crystals having mixed stack packing and long spin relaxation times: Tetramethylphenylenediamine (TMPD)/ tetracyanoquinodimethane (TCNQ), Naphthalene/1,2,4,5-Tetracyanobenzene (TCNB) and perylene/2,2'-Benzo[1,2-b:4,5-b']dithiophene-4,8-diylidene-bis-propanedinitrile (DTTCNQ).

In this study we were able to determine the criteria for charge transfer co-crystals with long spin relaxation times.

In addition, EPR study upon photoexcitation of Anthracene/TCNQ co-crystals showed the formation of spin polarized radical-pair spectrum and a spin polarized triplet spectrum. The triplet state had an ESP pattern of (a, e, e, a, a, e), this spin polarization phase pattern is a unique indication of spin selective charge recombination of a triplet RP precursor formed by the RP – ISC mechanism.

ORAL SESSION

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110 Spin Dynamics of SCRPs in ZnO Quantum Dot – Organic Molecule Conjugates.

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Photogenerated spin-correlated radical pairs (SCRPs) are emerging as promising new candidates for Quantum Information Science (QIS) applications where they act as electron Spin Qubit Pairs (SQPs). Historically, these pairs have been mostly investigated in natural photosynthesis and in molecular organic donor-(linker)-acceptor systems. However, recently we have shown that these spin pairs can also be observed by time-resolved Electron Paramagnetic Resonance (EPR) spectroscopy in hybrid inorganic-organic conjugates. In the current study we systematically prepare hybrid inorganic-organic molecule systems with tunable geometries that can host SCRPs/SQPs. The organic component based on 9,10-bis(phenylethynyl)anthracene acts as both chromophore and electron donor. Its design can be adjusted by synthetically changing the linker length and thus the distance to inorganic ZnO quantum dots (QDs) of various sizes, which act as electron acceptors. The range of resulting geometries allows for tuning of the electronic coupling and magnetic interactions. Here, we demonstrate using pulsed

EPR spectroscopy that we can generate, study and manipulate the spins in these photogenerated SCRPs hosted on highly tailorable inorganic-organic hybrid systems. An attractive feature of this class of hybrid materials is that the g-factor of the electron spin in ZnO QD (as part of the SCRP/SQP) can be adjusted using the quantum size effect in these QDs, which allows for selective addressability of each spin in the SCRP using microwave pulses that could open a door to advanced Quantum Information Science (QIS) applications.

ORAL SESSION

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111 Spin Dynamics in Singlet Fission Oligomers and Polymers with Tetracene Pendants.

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Singlet fission (SF) presents a viable avenue for surpassing the Shockley–Queisser limit in single-junction solar cells. In addition, SF also offers a promising approach to generate pure spin states in molecular systems, which is an essential requisite for quantum sensing and computation. Intermolecular SF has been detected in various organic materials; however, achieving highly efficient intramolecular SF faces hurdles such as competitive triplet–triplet recombination or nonradiative decay channels. Polymers, with their solution processability, excellent charge transport, and tunable microstructure, hold significant potential for enabling efficient intramolecular SF. Here, we employ time-resolved continuous wave (cw) and pulsed electron paramagnetic resonance (EPR) spectroscopic techniques to investigate key intermediates of SF processes in tetracene-pendent oligomers and polymers. The evolution and transformation of triplet and quintet spin states are explored as functions of oligomer length. Rabi nutations allow identification of spin multiplicity, and pulsed EPR spectra obtained at different delay times after the Laser flash (DAF) allow visualization of spin transformations. Our findings reveal that exciton translational motion along the pendent groups enhances the dissociation of triplet pairs, with oligomer length playing a critical role in modulating spin state interconversion and exciton transport. This work advances our understanding of SF in polymers, paving the way for their application in quantum information science and energy conversion technologies.

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112 Organic Molecules as Spin-optical Interfaces: From Magnetic Sensing to Photoredox Catalysis.

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The transduction of quantum information from the microwave to the UV-visible range can be surprisingly robust in open-shell organic molecules. At the heart of this possibility is the observation that small changes in spin dynamics can lead to drastic changes in electronically excited processes. In my talk, I will describe our recent efforts designing organic molecules whose ground-state properties can be exploited for magnetometry, serving as organic analogues of NV centers; some of the predictions have been demonstrated by recent experiments of the Wasielewski group. These examples provide clear evidence that chemical design can serve to augment the toolbox of quantum information. Conversely, I will conclude by suggesting that the opposite should also be true: subtle control of spin dynamics should lead to dramatic changes in chemical behavior in appropriately designed schemes for photoredox catalysis, and in particular, for enantiopurification.

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ORAL SESSION

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113 Heisenberg and Dipolar Spin Exchange Among Paramagnetic Probes in a Percolation Network.

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The rate of spin exchange among paramagnetic probes diffusing in a percolation network deviates from the linear concentration dependence that is observed in isotropic solutions. This effect is experimentally demonstrated for the Tempone spin probe in the aqueous phase of the hydrated ion exchange membrane Nafion 117. The observed EPR spectra are analyzed in terms of the new paradigm for interpreting spin exchange effects recently proposed by Salikhov[1] as well as by fitting the lineshape with the stochastic Liouville equation as implemented in the EasySpin package.[2] Differences between the effective spin exchange measured from the spectrum by these methods are compared and a physical interpretation of the features that appear in the spectrum at high exchange rates is presented. The results indicate that dipolar interactions contribute significantly to spin exchange in this system and reflect a high rate of probe re-encounters within the channels of the membrane. The nonlinear concentration dependence of spin exchange is paralleled by the non-classical decay kinetics of nitroxide disproportionation in acidified membranes. The results are discussed in terms of currently available models for diffusion and reaction in a percolation network and provide an estimate of the fractal dimension of the aqueous membrane phase. Supported by NSF grants DBI 32001 and CHE 0443616

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ORAL SESSION

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114 EPR Spectroscopy of Chiral Polyacetylene Thin Films.

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Chiral semiconductor materials have recently garnered significant attention due to their potential to enable spin-polarized charge transport without magnetic fields, as described by the chirality-induced spin selectivity (CISS) effect[1]. This emerging paradigm promises new routes toward low-power spintronic devices and quantum sensing platforms. Within this context, polyacetylene represents a prototypical organic semiconductor and conjugated polymer, known for hosting soliton charge carriers and exhibiting rich electronic structure dynamics[2]. However, traditional polyacetylene synthesized since the 1970s[3] has been regarded as achiral, at least macroscopically. Microscopically, it turns out that this material consists of an equal amount of fibrils with opposing chirality. This so-called racemic nature suggests that polyacetylene could actually be a true macroscopically chiral material when an imbalance of the fibrils with opposing chirality is achieved, opening up the potential to exhibit CISS-related phenomena. In this study, we have investigated the paramagnetic electronic states in polyacetylene thin films synthesized using a novel chirality-selective deposition technique. Circular dichroism and polarized Raman spectroscopy confirm the emergence of macroscopic chirality in these samples, in contrast to control films grown under racemic conditions, which show no net optical activity[4]. Continuous-wave electron paramagnetic resonance (cw-EPR) spectroscopy at room temperature reveals a key difference in the electronic structure of the two material types. While traditional racemic polyacetylene exhibits a single EPR resonance at g~2, chiral films show an additional, distinct resonance that is slightly shifted. This result suggests the presence of a new class of paramagnetic charge carrier states, linked to the chirality introduced during synthesis. Our findings imply that controlled induction of chirality in organic semiconductors can fundamentally alter their electronic spin structure, potentially enabling new pathways for spin-selective charge transport in polymer-based systems.

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ORAL SESSION

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115 Insights into Triplet Vinylidenes: Electronic Structure and Stability Using Imidazopyridine Scaffolds.

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Organic radical species have long been fundamental to chemistry due to their unique and strong reactivity. Vinylidenes, considered exotic analogues to carbenes, have been proposed to play a crucial role in numerous reactions, yet remained elusive until our group demonstrated the existence of a new class of stable ground-state triplet vinylidenes.[1,2] Similar principles have guided our recent exploration of a phosphorus-based vinylidene analogue,[3] underscoring the versatility of triplet-state stabilization strategies. Building on these findings, we now present the characterization of a novel triplet vinylidene species based on an imidazopyridine (IP) scaffold. Remarkably, small structural variations within these IP systems lead to dramatic changes in stability, ranging from unusually stable to the lower limit of stability for isolable triplet vinylidenes. In light of ongoing broad investigations into vinylidene stability, this wide stability range makes them excellent reference points for computational studies aimed at understanding vinylidene reactivity. To investigate how structural variations influence the stability of triplet-vinylidenes, we recorded pulsed EPR experiments at cryogenic temperatures. These data provided zero-field-splitting parameters and enabled lifetime analysis. Isotope-labeling combined with orientation-selective ENDOR spectroscopy enabled the reconstruction of the complete hyperfine tensor of the reactive site. Coupled with DFT calculations, this approach offers an in-depth view into the electronic structure and reactivity of these novel compounds.

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ORAL SESSION

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116 Probing the Electrical Properties of Twisted Tetrathiafulvalene Thin-Films Using cwEPR.

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Tetrathiafulvalene (TTF) and its derivatives exhibit non-conventional optical and electrical properties.[1] As a result, the strong electron-donor TTF has been a cornerstone of the field of organic electronics. In recent work, optical activity has been imparted on polycrystalline TTF films by incorporation of a twisting agent, abietic acid. This modification results in a twisted TTF polymorph, exhibiting enhanced hole mobility.[2] Doping this polymorph with iodine further improves its conductivity through the oxidation of TTF. The temperature dependent conductivity of single crystal TTF iodine salts has been investigated previously, revealing conductivity in temperatures above 80 K result from a single spin species with large spin orbit coupling, as evidenced by its 180 G linewidth and 2.013 g-factor, to the iodine sublattice.[3] As part of this study we use a combination of conductivity measurements, variable temperature cwEPR and pulsed EPR at X-band to characterize the spin species that contribute to charge transport in iodine doped, twisted and non-twisted TTF thin films. The undoped non-twisted film exhibits an inhomogeneously broadened, 20 G wide, ESR signal at 296 K with a g-factor of ~ 2.011. As the twisted film is doped, two partially overlapping spin species with a Dysonian lineshape are observed, consistent with an increase in conductivity. The respective g-factors were determined to be ~2.017 and ~2.012. The increase in intensity of the EPR signal, due to doping, is incommensurate with the in-situ conductivity, suggesting the number of paramagnetic defects is not entirely responsible for the improved performance. The normalized intensity of the g ~ 2.017 species increases with temperature, suggesting thermal activation of the site. We

investigate the sources of spin-lattice relaxation and coherence properties of the identified spin species as a function of temperature, and we compare these results to the observed conductivity.

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ORAL SESSION

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117 Electron Spin Relaxation and Pulse Turning Angles of Lanthanide Complexes.

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Pulse field-swept echo-detection permit observation of wide lanthanide spectra that extend over thousands of gauss. EPR spin-lattice relaxation times were measured for seven lanthanide(III) ions bound to a phosphine oxide ligand (tris-(3,5-dimethoxyphenyl) phosphine oxide) that forms meridional pseudo-octahedral 6-coordinate complexes. EPR spectra and relaxation times are compared with previously reported results for lanthanides in aqueous solution, bound to the protein lanmodulin, and bound to the bio-inspired small-molecule chelator 3,4,3-LI-(1,2-HOPO).[1] The emphasis in this discussion will be on the g value and energy level information provided by the electron spin turning angle in pulsed EPR measurements of lanthanides. For example, samarium(III) requires about 20dB (100 times) as much incident microwave power to create a 90° pulse as do terbium(III) and erbium(III). The turning angles provide insight into the J values for the ground states.

The EPR spectra and relaxation times are sensitive to the coordination environment and are emerging tools for characterization of both small-molecule and biomolecule interactions with lanthanide ions. Both Kramers and non-Kramers ions will be discussed.

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ORAL SESSION

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118 What Governs Spin Decoherence in Condensed Matter?

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In quantum state superposition (coherence), which is important in quantum information processing, the lifetime is the most important parameter, and it is evaluated by the spin-spin relaxation time T_2 determined by pulsed ESR measurements. We systematically measure the spin-spin relaxation of many systems and attempt to organize and understand it in terms of various physical quantities such as dimensionality, spin concentration, and transfer integral. In addition, we are "exploring systems with high spin concentration and slow decoherence."

To extend spin-spin relaxation, the spin-lattice relaxation time T_1, which determines the upper limit of the coherence lifetime, must be long. When considering applications, evaluation at room temperature is essential, but at room temperature, lattice vibration is intense and T_1 becomes significantly faster. Transition metals maintain stable spins, but because of the large spin-orbit interaction, non-degenerate S=1/2 systems that are expected to have long spin-lattice relaxation times are expected to be candidate materials. In collaboration with several

synthesis researchers in Japan, we performed pulse ESR measurements on various candidate materials that are thought to have long coherence.
We performed pulsed ESR measurements and/or photo-induced time-resolved ESR in the X-band region. The measurement targets include porous materials such as polyoxometalates (POMs), metal-organic frameworks (MOFs), and one-dimensional organic conductors. We summarize these results and discuss strategies for developing systems with long spin coherence.

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ORAL SESSION

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119 EPR Characterization of Molten Salt Synthesized Erbium(III) Doped Yttria Nanoparticles.

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Molten-salt synthesized Er^{3+}:Y2O3 nanocrystals is a promising platform for quantum sensing due to desirable optical and magnetic properties. Through X-band CW-EPR experiments the Er^{3+} spin centers are shown to retain a spectrum consistent with systems along with the presence of Y_2O_3 crystal defect centers and impurities.[1] Pulsed EPR experiments were performed to determine relaxation properties and mechanisms including T_1 and T_m anisotropy, instantaneous diffusion, spectral diffusion, and temperature-dependent spin–lattice relaxation. Instantaneous diffusion measurements show a small impact on T_m. Temperature-dependent T_1 and T_m measurements from 4-7 K are consistent with a Raman process and electron-electron spectral diffusion.[2]

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ORAL SESSION

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120 Manipulation of Spins in Pulse EPR.

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Manipulation of spins in pulse EPR has several ultimate goals: identification and quantitation of spin species; determination of their physical structure; determination of low-lying vibrational or electronic states; measurement of spin dynamics and relaxation; and for quantum informatics. The response of spins to any applied field involves many spin properties relevant to these goals, but the response to an arbitrary excitation often involves many relevant and irrelevant parameters, inviting over-fitting and over-interpreting of data. Consequently, pulse sequences and experiments were developed with multiple pulses, each pulse having specific intensity, duration, frequency, and phase, to make the measurement depend on only a single spin parameter. A single, long microwave pulse has been used to study T_1, Rabi oscillations, and coherence lifetimes. Yet, the effect of a long pulse on the spin system also is known to depend on spectral diffusion, the spin quantum number **S** and its zero-field splittings, the homogeneity of $\mathbf{B}_1$, the anisotropic **g** tensor, inhomogeneous broadening of the spins, weak nuclear spin couplings giving ESEEM, molecular motion, and even chemical reactivity. In several experiments where a single, long microwave pulse is currently used, that long pulse can be replaced by a specific series of two or more pulses to make the measurement results depend nearly exclusively on a single parameter of interest, avoiding the dangers of under- or over-fitting the data. A pair of four-pulse experiments demonstrate this. One four-pulse sequence isolates the decay of spin coherence by refocusing other causes of Rabi oscillation decay, allowing accurate study of 'T_2' in the doubly rotating frame. The other four-pulse sequence measures g-factor anisotropy in disordered samples from Rabi oscillation measurements at a single magnetic field.

ORAL SESSION

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121 Structure and Dynamics of Monoclonal Antibodies using Spins, Scattering, and Simulations.

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Monoclonal antibodies (mAbs) are the leading biologic drug platform ($75B/year). These multi-domain proteins exhibit both intra- and inter-domain structural distributions important in modulating their on-target therapeutic and off-target toxic effects. Lack of quantitative information on these structural ensembles impedes innovation and development of novel biopharmaceuticals. To address this measurement problem, we have designed a means to derive biomolecular ensembles from distance distribution measurements via a library of spin-labeled proteins with high affinity for a target biologic. The NISTmAb reference material (NIST RM 8671) serves as our development platform for spin-labeled affinity protein (SLAP) reagents. Our SLAP reagents are compatible with any non-isotopically labeled immunoglobulin G class mAb derived from a mammalian expression system. Integrating molecular simulations with double-electron electron resonance

(DEER) spectroscopy and solution X-ray scattering measurements, we are simultaneously determining structural distributions and dynamics of mAb-based biologics (1).

(1) Szalai *et al.*, *ChemMedChem,* **2025**, 20, e202400917. https://doi.org/10.1002/cmdc.202400917

ORAL SESSION

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122 Nanotemplate Approach to Stabilize Macroscopically Aligned Lipid Bilayers and Membranes Proteins under a Broad Range of Temperatures and Hydration Levels.

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Magnetic resonance spectroscopy of macroscopically aligned samples provides a wealth of information and significantly improves resolution vs. polydisperse spin systems. The method is more developed for NMR of membrane proteins and remains less explored in EPR. The most employed alignment systems for NMR are (1) bicelles composed of mixtures of phospholipids and detergents and (2) macrodiscs formed by encircling fragments of lipid bilayers by amphipathic helical scaffold peptides or polymers. Both lipid mimetics exhibit a sufficient degree of magnetic susceptibility anisotropy to spontaneously align in a sufficiently strong magnetic field. However, sample temperature must remain at >30-35 °C with sample water content of at least 70-80v%. Once the temperature or water content is lowered the macroscopic order is. In contrast, the method we developed - self-assembled lipid nanotubular bilayers formed by self-assembly inside cylindrical nanopores of ca. 50-250 nm in diameter and composed of anodic aluminum oxide (AAO) – can retain the macroscopic order over an exceptionally broad range of temperature, pH, and salt concentration. Here we employed spin-labeling EPR at X- and W-bands (9.5 and 94 GHz) to validate the macroscopic alignment at both physiological temperatures and upon freezing down to cryogenic temperatures for both lipid bilayers and integral membrane proteins including large photosynthetic complexes for which the first orientation-dependent HYSCORE spectra were obtained. Next, we demonstrate that most of the water in the nanopores can be replaced by polysaccharides, so the lipid order is maintained even for mostly dry samples. Such an alignment approach significantly improves dipolar modulation amplitude in DEER of transmembrane proteins. Overall, macroscopically aligned minimally hydrated lipid samples immobilized in nanoporous matrices represent an attractive approach for preparing samples for room temperature mm-wave EPR and DNP NMR using high-Q photonic band-gap resonators we described previously.

ORAL SESSION

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123 Structural Identification of the Building Blocks of a Small Heterogenous Amyloid Oligomer by ESR.

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Amyloid oligomers represent an intermediate species in the aggregation of proteins involved mainly in neurodegenerative disease. Their structural characterization has been elusive due to their transient and heterogeneous nature. One amyloid oligomer that has been solved by X-ray crystallography is of a small model peptide called K11V.[1] So far, ESR measurements have characterized the aggregation of the oligomer by size,[2] but distance measurements have been difficult due to the propensity of spin labels to inhibit oligomerization, and the potential for multi-spin and overlapping distance distributions. Using a bifunctional spin label, we were able to spin label K11V in a manner that allows the oligomerization of the peptide, and labels the peptide in-range for distance measurements. Previously, T1-edited DEER measurements (iDEER) have been shown to separate complex distance distributions by the number of spins,[3] but we have shown that relaxation-filtering is also distance-dependent. We have filtered distances in the distance distribution from spin-labeled K11V, allowing the further identification of distances belonging to the hexameric K11V building blocks, and distances belonging to higher-order oligomers. This work shows that small beta-sheet-rich amyloid oligomers are accessible by ESR distance measurements.

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ORAL SESSION

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124 Tuning Sidechain Protonation at the Membrane Interface: Implications for T-Cell Receptor Assembly.

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The ionization states of amino acid residues are critical for membrane protein assembly and function, yet they remain challenging to resolve experimentally. This difficulty is amplified in membrane proteins due to limited data on transmembrane gradients in polarity, electric potential, and hydration at the protein-lipid interface. In this study, we investigate how electrostatic interactions—previously implicated as key drivers in the membrane assembly of the T-cell receptor (TCR)—can be modulated through changes in membrane lipid composition. To probe these interactions, we employed novel pH-sensitive, ionizable electron paramagnetic resonance (EPR) spin labels to map the heterogeneous dielectric environment along transmembrane protein-lipid interfaces. Using a series of model transmembrane ?-helical WALP peptides, we established the depth-dependent profile of effective pK? values across the membrane. Our findings demonstrate that the effective pK? of ionizable sidechains embedded in the membrane interior can be significantly shifted by altering the surface charge density of the lipid bilayer.

To explore the biological relevance of these observations, a pH-sensitive nitroxide-labeled peptide corresponding to the transmembrane domain of TCR? was incorporated into liposomes. EPR measurements provided insights into the sidechain's protonation state, membrane insertion, and helix-helix interactions. Increased negative surface charge on the membrane was found to modulate the protonation state of buried ionizable residues, influencing transmembrane domain association. Using Double Electron-Electron Resonance (DEER) spectroscopy, we demonstrated that neutralizing the charge of an ionizable sidechain enhanced the tendency of transmembrane domains to cluster—an effect likely important in TCR assembly and turnover.

EPR spectroscopy using ionizable probes offers a powerful method for elucidating how local environmental changes at protein-lipid interfaces can fine-tune the pK? of ionizable residues and drive structural dynamics in membrane proteins. This material is based upon work supported by the National Science Foundation under Grant No.2305172.

ORAL SESSION

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125 Development of EPR Technologies to Elucidate Signaling Selectivity in GPCRs.

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G-protein coupled receptors (GPCRs) are a large and diverse class of cell surface receptors responsible for regulating nearly every physiological process in the human body and have long been important targets for drug development. Many GPCRs signal through several pathways that include different G-protein subtypes and arrestins, and designing drugs that can preferentially activate or suppress a specific pathway is a major frontier in structure-based drug design. To achieve this goal and define the molecular mechanisms of ligand-mediated signaling, it is necessary to identify functional conformational states whose equilibrium populations are modulated by ligands with distinct efficacy profiles and to delineate the role of conformational dynamics in regulating receptor signaling. Site-directed spin labeling coupled with EPR (SDSL-EPR) is a particularly attractive in-solution measurement for elucidating protein conformational landscapes because it is applicable under physiological conditions, has no protein size or complexity restrictions, and has high sensitivity for detection (picomoles-nanomoles). I will present recent EPR technology development efforts in my lab, all of which were designed for applications in GPCR conformational efficacy and time-resolved conformational dynamics. We developed a novel platform to model conformational ensembles using DEER-derived distance constraints in guided MD simulations. In an initial application using published data on the angiotensin 1 type II receptor (AT1R) – one of the most widely studied GPCRs and a prime target of cardiovascular therapeutics – we identify distinct structural models stabilized by balanced and pathway-selective ligands and uncovered a novel ?-arrestin selective conformation, providing mechanistic insight into the pathway-specific efficacy in AT1R. I will also present two different systems we developed to access ms-timescale conformational fluctuations in complex, biomedically relevant proteins such as GPCRs: a complete high-pressure EPR system at Q-band for both static pressure and pressure-jump measurements, and a high-sensitivity stopped-flow EPR system at X-band.

ORAL SESSION

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126 In-cell Cu(II)-NTA Labeling for EPR Distance Measurements.

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To gain an holistic understanding of protein function, structure and dynamics measurements must be carried out in-cell to account for molecular and physical crowding effects. Recent developments in EPR methodology have revealed the power of this technique to measure structural constraints in-cell. However, there remains a serious bottleneck, as proteins must be labeled ex-situ or using noncanonical amino acids. In this work, we expand current endogenous labeling methods using the Cu(II)-NTA spin label, quantify the amount of spin label delivered into the cells, assess spin labeling, and account for orientational effects during distance measurements.1 Additionally, we show that hypotonic swelling is a reliable method deliver Cu(II)-NTA into cells, achieving a bulk average of 57uM spin labeled site across six repeats. Our work provides a way to circumvent the current endogenous labeling bottleneck, making in-cell spin labeling accessible to the broader EPR community.

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ORAL SESSION

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127 Rigid Cu(II) Spin Label Sensitive to DNA Conformational Flexibility in Protein-DNA Complexes.

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Measuring DNA conformation in protein-DNA complexes is essential for understanding how DNA structure and dynamics influence protein recognition and function. In this work, we introduce a new nucleotide-independent labeling strategy wherein Cu(II) is introduced directly within the DNA helix. The strategy utilizes two 8-

aminoquinoline groups, one of each strand that rigidly anchors the Cu(II) ion within the DNA. The rigidity of the label allows us to accurately measure DNA conformations and dynamic fluctuations without convolution due to flexing of the label itself. To demonstrate the utility of the new label, we measure the changes in conformation of DNA when it binds to type II restriction endonuclease EcoRV. The findings offer direct evidence in solution that the EcoRV endonuclease causes axial bending of DNA even without metal ions. Additionally, the narrowing of the distance distribution upon protein binding—and further with metal ion binding—suggests that the protein restricts the flexibility of the DNA helix. This approach presents a new and precise method to analyze DNA structure and dynamics in solution.

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ORAL SESSION

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128 Photochemical and Mechanical Activation of Metal Oxide Additives Drives Radical Formation in Lubricating Oils: an EPR Spin-Trapping Study.

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Nanoparticle (NP) additives have recently attracted considerable attention for their ability to enhance the tribological and thermophysical properties of petroleum-based lubricants. However, relatively little research has explored their potential to generate free radicals in oils through photochemical or mechano-activation mechanisms.

In this study, spin-trapping Electron Paramagnetic Resonance (EPR) spectroscopy was employed to quantify and characterize short-lived free radical intermediates formed in light mineral oil (LO) containing nanoparticles. Upon photoactivation with 365 nm UV light, TiO?, CeO?, and Zn nanoparticles significantly increased radical production compared to oil-only controls, particularly when molecular oxygen was present. TiO? and CeO? primarily promoted the formation of alkoxyl radicals, while ZnO favored peroxyl radical generation in air-equilibrated samples. In contrast, in the absence of oxygen, the presence of nanoparticles had little to no effect, or even a suppressive effect, on radical formation, primarily due to reduced generation of carbon-centered radicals. These results underscore the critical role of molecular oxygen in radical formation initiated by photochemically active nanoparticles.

Mechanoactivation of metal oxide nanoparticles, achieved by milling, led to surface modification of TiO? particles, as evidenced by the detection of stable radical species via low-temperature EPR. When added to air-equilibrated LO, mechanoactivated TiO? particles induced the formation of both alkoxyl and peroxyl radicals, with peroxyl species being predominant. Extending milling time beyond 30 minutes resulted in a modest increase in radical production. Notably, the mechanoactivated TiO? retained approximately 25% of its radical-initiating activity even 24 hours after milling, indicating persistent surface reactivity. The effects of mechanoactivated ZnO and alumina particles on radical formation in LO are also examined and discussed.

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ORAL SESSION

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129 Flavoproteins as Native and Genetically Encoded Spin Probes for in Cell ESR Spectroscopy.

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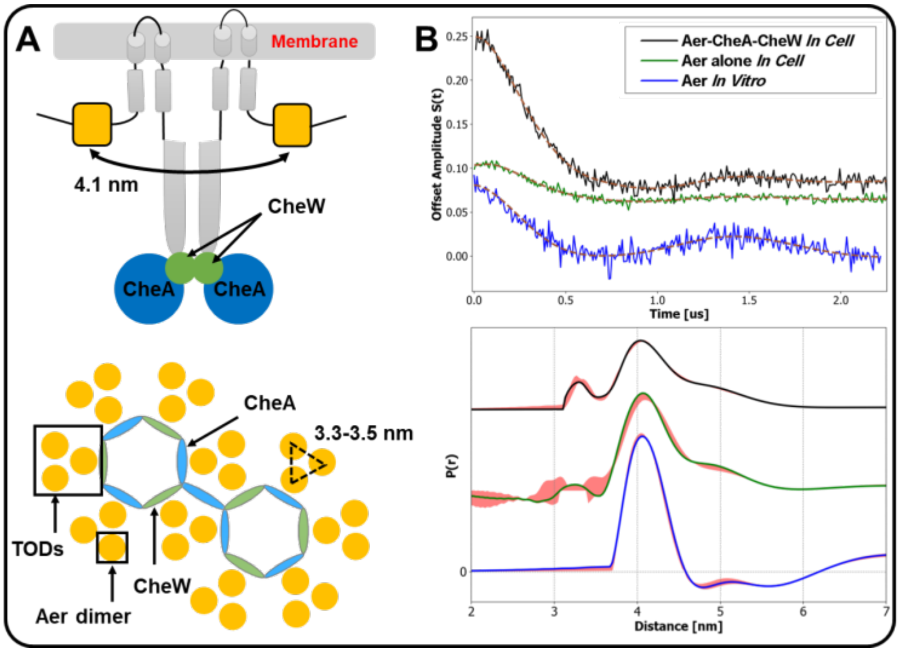
The use of spin probes has been limited by their permeability and their chemical stability in cell. To overcome this challenge, we developed a new category of spin labels that are based on flavoproteins. We studied the transmembrane receptor Aer as a model system containing stable flavin radicals *in vivo* and we elaborate a genetically encoded flavoprotein domain iLOV as a spin label that could be

expressed genetically and attached directly *Escherichia coli* (*E. coli*) to a protein of interest.

Most mobile bacteria move towards favorable environments by exhibiting a behavior known as chemotaxis[1]. In *E. coli*, Aer is a primary energy sensor for mobility. Aer responses are determined by the redox state of the flavin adenine dinucleotide (FAD) cofactor, which sends signals from the electron-transport chain to the chemotaxis histidine kinase CheA[2]. Aer has been previously studied by electron spin resonance (ESR) in reconstituted systems with membranes or nanodiscs[3]; however, such systems do not recapitulate the higher-order assembly states chemoreceptors that Aer likely form to amplify signals.

In this study, we optimize biochemical and spectroscopic conditions to investigate Aer and obtain insight by 4P-DEER on the organization of Aer in chemosensory arrays. In parallel, we bioengineer a flavoprotein domain iLOV and fuse it to CheA, revealing domain associations that only occur *in vivo*. Whole cell isotopic labeling (^{2}H or ^{15}N) is also carried out to improve the distance range measurement obtained by 4P-DEER and to achieve the complete characterization of the spin system by cw-ESR and hyperfine pulsed ESR spectroscopy. These live-cell studies have the potential to reveal signaling features of proteins involved in chemotaxis. This research has been submitted to Nature Communication[4] and is supported by Supported by NIH R35GM122535 (BRC) and NIH R35GM148272 (JHF) and R24GM146107, P41GM103521 (JHF & BRC).



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ORAL SESSION

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130 EPR and FIRMS Characterization of the Magnetic Anisotropy in a Set of Metalorganic Mn^{III}[R-sal$_2$323]$^+$ Spin-Crossover Complexes.

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Certain octahedrally coordinated 3d^4-3d^7 transition metals can undergo spin-crossover (SCO) transitions between a low spin (LS) and high spin (HS) state in response to external stimuli such as temperature, light, pressure, and magnetic or electric fields. Owing to strong spin-lattice coupling, a spin state transition at one site induces local lattice strains that quickly propagates the spin state transition to neighboring sites. This cooperative behavior allows significant change in magnetic susceptibility to be triggered by relatively minor external perturbations, making such systems highly promising for a range of applications.[1] In this investigation, we focused on synthesizing mononuclear Mn^{3+} complexes coordinated with a hexadentate Schiff-base ligand (R-sal$_2$323) which facilitates stabilization in the LS state and promotes SCO behavior. Our aim was to study the magnetic anisotropy and SCO behavior of these complexes upon systematically modifying the R-substituents on the sal$_2$323 ligand, changing the counterions, and incorporating solvent molecules into the crystal lattice. To characterize the zero-field splitting (ZFS) parameters and the g anisotropy associated with the spin quintet (S = 2) and triplet (S = 1) states, we employed continuous-wave high-field electron paramagnetic resonance (cw-HFEPR) and far-infrared magnetospectroscopy (FIRMS) techniques on both powder and single-crystal samples. The SCO behavior was further investigated using superconducting quantum interference device (SQUID) magnetometry. A comparative analysis revealed that while the SCO behavior was significantly influenced by the structural modifications, the magnetic parameters exhibited less sensitivity to these changes. Notably, the positive ZFS parameters observed in both the HS and LS states suggest an unusual ligand-driven axial compression across all studied complexes. These findings underscore the pivotal role of the Schiff base sal_2323 ligand in the electronic and geometric structure in this family of Mn^{3+} complexes.

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ORAL SESSION

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131 Electronic Wavefunction Delocalization Beyond the Metallic Core of Palladium Dodecanethiolate Nanoparticles: Revealed through Pulse ESR.

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Ligand-stabilized metallic nanoparticles exhibit diverse functionality across catalysis, sensing, and biomedicine driven by the behavior of itinerant electrons. The electrons delocalized nature give rise to the most desirable properties of nanoparticles such as their conductivity, high density of states, and enhanced polarizability. These attributes are often conceived as characteristics of the core which is distinct from the ligand and solvent shells. However, there is scant research exploring the extent of the metallic core wavefunction delocalization into the surrounding chemical environment. The electron and nuclear spin couplings of palladium dodecanethiolate nanoparticles has been discovered through pulse

electron spin resonance. Systematic exploration of labeled and unlabeled ligands and solvent demonstrated that both nuclear spins from the thiol and solvent were coupled to the electron spin of the metallic core. Thus revealing the metallic electrons are not isolated to the core, but rather extend through-space interactions. These preliminary results serve as a basis to begin further investigation into directed tunability of the metallic wavefunction propagation for controlled functionality.

ORAL SESSION

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132 Lessons from Preclinical EPR pO2 Oxygen Images.

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We have previously presented data from spin lattice relaxation (SLR) rate pO2 images from OX071 trityl spin probe delivered intravenously to tumors in mice to locate hypoxic tumor grown in their legs, defined as pO2<=10 torr using 250 and 720 MHz EPR imagers. The images, registered with an isocentric radiation delivery system, were validated in three tumor models directing radiation boosts to greater than 98% of the hypoxic tissue and comparing the effectiveness of these hypoxic boosts to well oxygenated boosts of equivalent integral dose volume regions. This demonstrated a doubling of tumor control from the hypoxic boosts relative to the tumor control from the well oxygenated boosts, all of which were delivered after a 15% or 20% tumor control dose (the ankle in the logistic dose vs tumor control curve measured separately) providing the first mammalian a biologic validation of cancer treatment enhancement from targeting hypoxic tumor. A novel PET-EPR imager provided registered 18Fluoromisonidazole (FMiso) images and provided an opportunity to compare nitroimidazole PET with validated SLR pO2 EPR located hypoxia and use dynamic contrast enhanced (DCE) to correct the PET(in progress). Finally, an in vivo oxygen enhancement ratio, defining the correct amount of extra radiation that produced measurable enhancement of tumor control has been completed and suggests that work in patients with tumor hypoxia defined by PET underdosed the boost, but not by the large extra doses suggested by cellular measurements.

ORAL SESSION

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133 ACERT: A Service Resource for ESR Researchers

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This talk will focus on the various ESR technologies available at National Biomedical Resource for Advanced Electron Spin Resonance (ESR) Spectroscopy (ACERT) and how the ESR community can benefit from such resources, from instrumentation to sample preparation to data analysis. ACERT promotes the application of cutting-edge instrumentation and techniques to some of the most challenging questions confronting molecular biologists, as well as the expertise of ACERT personnel and the administrative leadership team to provide support to molecular biologists using the facility. More specific goals include 1) to provide facilities for protein structure determination by pulse dipolar ESR (PDS); 2) to provide facilities for study of real-time dynamics in biological systems (2D-ELDOR); 3) to provide facilities for more standard ESR experiments, but at a wide range of frequencies; 4) to provide unique data analysis methodologies to the world-wide community; 5) to fulfill training and outreach roles; 6) to provide the needed administrative support. Our NIH-funded ACERT has been in existence since 2001 and is home to world-class ESR spectrometers with well-organized facilities and a solid record in addressing protein structural and dynamics issues using many ESR methods. In its new avatar as a service center, many ESR technologies developed and hosted at ACERT that is now available to ESR community. We are providing training on the new concepts and on the use of the latest spectrometers, software, and their capabilities, and making them available to the community as users and/or for us to run the samples, analyze them, and supply the useful results to the community. Since ACERT is funded by the NIH, the services we provide are mostly free of charge.

ORAL SESSION

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134 Shallow Donors in Hexagonal Silicon Carbide: A Qubit Candidate Investigated by Pulsed EPR and Pulsed ENDOR at High Field.

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Since the proposal by Bruce Kane to use shallow donors in silicon for quantum computations[1], defects in semiconductors have attracted great attention in the quantum information context. Coherence times in sparse nuclear spin environments can be very long and in principle allow thousands of quantum operations before the coherence is lost. Now limited quantum computing can be achieved in systems based on phosphorus in silicon and also NV centers in Diamond. Here we focus on the closely related nitrogen impurities in hexagonal silicon carbide, which energetically are very similar to the Si:P system. The situation is more complicated due to the lower symmetry and the presence of more than one type of nitrogen substitutional center, which constitutes a challenge as well as an opportunity. Here we present high field pulsed ENDOR of the hexagonal nitrogen site in natural abundance 4H-SiC in an effort to describe the extended wavefunction. Also we present the T_1 and T_2 spin relaxation characteristics of both the hexagonal and the cubic center in 4H-SiC, which shows a marked field/frequency dependence due to the increasing phonon-density of states with frequency. At the highest frequencies the coherence time of the hexagonal center starts to be limited by the spin-lattice relaxation. The National High Magnetic Field Laboratory is supported by the NSF through DMR-2128556 and the State of Florida.

B. Kane, Nature, 1998, 393, 133.

ORAL SESSION

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135 Optical Detection of Carbon-13 NMR in Diamond for Rotation Sensing.

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We investigate the use of ^{13}C nuclear spins in diamond as a candidate system for nuclear magnetic resonance (NMR) based rotation sensing. The high density and relatively weak gyromagnetic ratio of ^{13}C nuclear spins afford favorable properties for rotation sensing, including relatively long spin dephasing times and robustness against ambient field and temperature fluctuations. Moreover, ^{13}C spins in diamond can be initialized to a high degree of spin polarization using optical and microwave interrogation. However, detection of ^{13}C NMR in diamond has so far relied on inductive detection, which has relatively poor sensitivity at the low magnetic fields required for rotation sensing. Here, we demonstrate a technique that takes advantage of microwave-swept “Landau-Zener” crossover resonances to transfer spin quanta between Nitrogen-Vacancy (NV) electron spins and ^{13}C nuclear spins via their transverse hyperfine interaction,[1,2] allowing for both optical hyperpolarization and readout. We perform optically-detected ^{13}C Ramsey spectroscopy and realize a ^{13}C-spin-dependent fluorescence contrast approaching 1%, with dephasing time T_2^*? 2 ms. We study the magnetic field dependence of the optical readout and find good performance for magnetic fields below 10 mT. Our method can be interpreted as a type of repetitive readout where each NV center is used to read out the spin state of hundreds of ^{13}C nuclei before nuclear spin relaxation processes dominate. We show that this property offers a commensurate improvement in sensitivity compared to gyroscopes based on the ^{14}N nuclear spins associated with NV centers.[3]

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2. Ashok Ajoy *et al.*, Orientation-independent room temperature optical 13C hyperpolarization in powdered diamond. *Sci. Adv.* **4**, eaar5492 (2018).

3. Andrey Jarmola *et al.*, Demonstration of diamond nuclear spin gyroscope. *Sci. Adv.* **7**, eabl3840 (2021).

ORAL SESSION

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136 Optically Detected Coherent Spin Control of Organic Molecular Color Center Qubits.

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Molecular optical-spin interfaces are emerging as promising alternatives to solid state defects such as diamond nitrogen vacancy centers for quantum information science applications.[1,2] In this work, we report an optical-spin interface in organic molecular qubits consisting of two luminescent tris(2,4,6-trichlorophenyl)methyl (TTM) radicals connected via the *meta*-positions of a phenyl linker.[3,4] Optical polarization of the $|T_0\rangle$ sublevel of the triplet ground state is achieved by spin-selective excited-state intersystem crossing from the $|T_+\rangle$ and $|T_-\rangle$ sublevels of the triplet excited state. Addition of a methyl substituent to the phenyl linker increases the predicted excited-state intersystem crossing spin selectivity from 80% to 97% while reducing the electronic coupling between the TTM subunits. This is supported experimentally by an order of magnitude increase in the optically detected magnetic resonance contrast and longer excited-state lifetimes. We demonstrate coherent microwave manipulation of the spin polarized ground state populations and coherences using optically detected Rabi nutations, Hahn echo formation, and echo decay measurements at 85 K in a nuclear-spin rich solvent matrix. This marks a crucial step towards leveraging the favorable spin relaxation times of organic molecules for applications as quantum sensors at temperatures that heretofore have been difficult to achieve by molecular color centers. In addition, we demonstrate that the optical-spin interface of organic diradicals is preserved in doped crystals with favorable spin relaxation times up to room temperature, which is promising for the development of next generation quantum sensors.

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ORAL SESSION

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137 Anisotropies of Electrically Detected Multiphoton EPR Transitions in the Nonperturbative Resonant Drive Regime.

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The Floquet theory-based description of electron paramagnetic resonance (EPR) in the nonperturbative regime—when the amplitude $B1$ of the radiofrequency magnetic resonant drive-field is approximately equal to or in excess of the static magnetic field $B0$—predicts the emergence of various dressed electron spin states [1-3]. These Floquet states appear to be good candidates for solid state quantum bits due to their expected long coherence times and potential electrical single spin readability [4,5]. In order to test Floquet theory, we have conducted strong-drive EPR experiments in the regimes where $B1 > 1$ mT and $B0 < 2$ mT, using room temperature, low magnetic field, electrically detected magnetic resonance (EDMR) spectroscopy of spin-dependent charge carrier (polaron) recombination currents in organic light emitting diode (OLED) structures whose active devices layers are based on either "Super-Yellow" (SY) poly(1,4-phenylene vinylene) (SY-PPV) or deuterated poly[2-methoxy-5-(2'-ethylhexyloxy)-1,4- phenylenevinylene] (d-MEHPPV). The focus of this work is to scrutinize Floquet theory-based predictions for multiphoton resonance signal magnitudes as a function of the angle θ between $B0$ and linearly polarized $B1$.

We performed EDMR spectroscopy on OLEDs with a 50 MHz resonator and showed that the angles θ at which signal maxima and minima occur experimentally agree with the predictions of Floquet theory for one-, two-, three- and even four-photon transitions, the last of which we have observed for the first time in our experiments.

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ORAL SESSION

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138 Dielectric Resonator Optimization for EPR Spectroscopy and solid-state MASERs.

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Microwave resonators in EPR spectroscopy concentrate and align the microwave magnetic field (B_1) and simultaneously separate the microwave electric field from the sample, preventing heating. There are numerous experimental methods in EPR spectroscopy which impose different requirements on MW resonators (e.g. high or low quality factor, microwave conversion, and B_1-field homogeneity). Although commercial spectrometers offer high performance standardized microwave resonators for a broad application range, emerging and highly-specialized research fields, such as masers[1], require even better sensitivity. Here we low-cost optimization approaches for a commercially available X-band (9–10 GHz) MW resonator which improved the performance in terms of conversion, microwave field homogeneity and Quality factor[2]. Our results demonstrate that small changes to a microwave resonator can enhance its performance in general for EPR spectroscopy and for specific applications, such as solid-state masers[3] in particular.

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ORAL SESSION

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139 A Free-electron-laser-powered Agile Pulsed Electron Spin Resonance (FEL AESR) Spectrometer.

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Driven by scientific opportunities in condensed matter physics, quantum information science, chemistry, biology, and engineering, worldwide efforts are expanding pulsed electron magnetic resonance spectroscopies to ever higher static magnetic fields, microwave frequencies, and microwave powers. For studies of spin relaxation times in many systems—for example, molecules with large zero-field splittings, or fermionic collective excitations in quantum magnets—it is highly desirable to develop the capability to perform pulsed ESR experiments at sufficiently high power to resolve ns relaxation times while operating over a wide range of frequencies above 100 GHz and high magnetic fields. At UCSB, a unique pulsed ESR spectrometer that is designed to measure ns spin relaxation times at magnetic fields up to 16 T at frequencies tunable between 170 and 420 GHz and temperatures of ~2 to 300K is nearly complete. The design and performance of subsystems and the assembly will be described in this talk. The microwave sources are amplifier-multiplier chains (AMC), and one of the UCSB free-electron lasers (FEL). The FEL can generate kW powers for a few microseconds, or 10s of kW in 40 ns pulses when cavity-dumped. Three broad-band stacked complementary-channel pulse slicers,1 separated by two phase shifters, enable slicing the FEL output into up to three kW microwave pulses with independently controllable duration, phase, amplitude and power. A novel quasi-optical circuit will enable operation in three modes with only small user adjustments: using the sliced FEL pulses; using the AMC for cw ESR, and pulsed ESR on systems with relaxation times longer than a microsecond; and two-color experiments like spectral-hole burning, in which a FEL pulse is used as pump and the AMC output is used as a delayed probe at a different frequency. Initial science targets will be described. This work is supported by NSF DMR 2117994.

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10.1063/5.0180412.

ORAL SESSION

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140 Multi-Extreme THz ESR: Past and Future.

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Related to the receipt of the IES Fellow, I would like to overview our developments of multi-extreme THz ESR.[1] We have been developing THz ESR under multi-extreme conditions, such as high magnetic field, high pressure and low temperature in Kobe. It covers the frequency region between 0.03 and 7 THz,[2] the temperature region between 1.8 and 300 K,[2] the magnetic field region up to 55 T,[2] and the pressure region is extended from 1.5 GPa[3] to 2.5 GPa using the hybrid-type piston-cylinder pressure cell.[4] It also includes mechanically detected ESR[5] measurements using a commercially available membrane-type surface stress sensor, which is the extension from our micro-cantilever ESR[6]. Finally, as an example, application of high pressure THz ESR to understand the pressure-induced phase transition in the Shastry-Sutherland model substance $SrCu_2(BO_3)_2$ will be discussed. Using our technique to observe the first excited state, we were able to determine the pressure where the pressure-induced phase transition occurs, and obtain the pressure dependence of exchange interactions in $SrCu_2(BO_3)_2$.[7] Comparison of our results with the theory will be discussed.

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ORAL SESSION

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141 Non-Uniform Sampling for Pulsed Dipolar Electron Spin Resonance Spectroscopy.

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Pulsed Dipolar Electron Spin Resonance Spectroscopy (PDS) is a uniquely powerful technique to measure the unbiased shaped of distance distribution P(r) between two radicals (i.e., those containing unpaired electron spin(s))[1,2]. However, PDS study time takes several hours to obtain a single trace. There are multiple methods to reduce data collection time by increasing the signal-to-noise (SNR) reducing signal averaging time, such as raising the RF power, increasing sample concentration, solvent deuteration[3], protein deuteration[4] or wavelet denoising[5]. Here we introduce another approach to reduce the data collection times by employing non-uniform sampling in PDS experiments. By selectively sampling time-domain points based on their contribution to distance distribution P(r) rather than uniformly, non-uniform sampling significantly reduces data acquisition time without compromising the quality of the reconstructed distance distribution P(r). Our implementation of non-uniform sampling on DEER data successfully reconstructs the distance distribution P(r) within the 95% uncertainty range of the reconstruction obtained from fully sampled data, while requiring 30%-40% of the data. This approach can enhance experimental throughput, approximately reducing data collection time for Q-band by 7-8 hours for a data collection time of 12 hours, and for X-band by 20-28 hours (for standard data collection time: 40 hours). Additionally, this methodology can be used in combination with the aforementioned time reduction techniques to further reduce the data collection time.

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ORAL SESSION

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142 Following Conformational Changes in LbuCas13a from Apo to the Ternary Complex with PELDOR.

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The type VI CRISPR effector protein Cas13a is an RNA nuclease, catalyzing two RNA cleavage events: First, the maturation of pre-crRNA and second, the cleavage of target RNA, activating a non-specific, collateral cleavage.[1,2]Although all four structures of Cas13a on route from apo, via the pre-crRNA bound complex (Cas13a-precr), the crRNA bound complex (Cas13a-cr), and the crRNA-target RNA bound complex (Cas13a?cr+target) are known, they origin from proteins of different organisms and contain different extends of truncation. To identify and follow conformational changes on a molecular level, structures of Cas13a in all states from one organism are needed. We aim to follow conformational changes by site-directed spin labelling in combination with Pulsed Electron-Electron Double Resonance (PELDOR or DEER) spectroscopy, which enables measuring distance distributions between spin labels in e.g., biomolecules in the range of 1.6-16 nm.[3]

To this end, we choose Leptotrichia buccalis (lbu) Cas13a for which the structures in complex with crRNA and crRNA/targetRNA are known, whereas the structures of the apo and precrRNA-bound complexes are unknown. We labelled lbu Cas13a with pairs of nitroxide spin labels at different positions and tested their influence on the functionality. All active constructs were subjected to PELDOR experiments. We compared the resulting distance distributions with and without RNA to in silico-generated distributions. These were calculated with the software mtsslWizard[4] and are based on the experimental RNA-bound structures as well as the AlphaFold2[5] structure as input. We show that the apo structure of lbu Cas13a has a very flexible and wide-open recognition lobe (REC-lobe). In contrast, the nuclease lobe (NUC-lobe) is preorganized. Upon pre-crRNA addition, a rigidification and conformational selection of the Helical-2 domain in the NUC-lobe occurs. The structure of the Cas13a-pre-crRNA complex is very similar to the known structure of lbu Cas13a-cr. The conformation and conformational changes between Cas13a?cr and Cas13acr+target fit to the known structures. In addition, our data suggest Cas13a dimerization in the presence of RNA.

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ORAL SESSION

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143 Breaking the Cycle: How Enzymes Control Oxygen Rebound for Versatile Biocatalysis.

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Fe/2OG enzymes catalyze numerous reactions in the biosynthesis of natural-product drugs. The active center of these enzymes consists of a single Fe(II) ion coordinated by a conserved set of amino acids (a so-called "facial triad"). Despite the simplicity of the metallocofactor, enzymes of this family show surprising diversity in the types of chemical reactions that they can catalyze. What governs this divergence of reactivity remains unknown, largely due to the fleeting nature of reaction intermediates. In this presentation, we show an Electron Paramagnetic Resonance (EPR)-based methodology that reveals the key structural differences among enzymes from different functional subclasses. This methodology deploys a stable and validated structural mimic of the key, conserved ferryl intermediate, V(IV)?O, [1] which is EPR-active and allows access to precise details about the surroundings of the metallocofactor using various pulse EPR methods, such as Hyperfine Sublevel Correlation spectroscopy (HYSCORE) and Double Electron-Electron Resonance (DEER). Using orientation-selective HYSCORE, we determine the proximity and the exact disposition of the strategically installed deuterons on relevant substrates and metallocofactors. Using this data, we show that in such cases as halogenases SyrB2[2,3] and WelO5, substrate-metallocofactor disposition is the key. In other cases, such as hydroxylase/oxacyclase H6H[5], the mode by which the reactivity is diverted is far more subtle and requires exact substrate positioning. Furthermore, we will discuss the possibility of resolving the structural mobility of the V(IV)?O bond with respect to protein using orientation-selective DEER in combination with site-specific spin labeling. Supported by NIH GM141284.

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ORAL SESSION

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144 Complete Expressions for Accurate Simulations of Strong and Weak-Pulse DQC and DEER Experiments.

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Double quantum coherence (DQC) and double electron electron resonance (DEER) spectroscopies are powerful pulsed dipolar spectroscopy (PDS) techniques for determining inter-spin distance distributions P(r). Coupled with site-directed spin labelling, these distance distributions are used for studying protein structures and protein−protein interactions. PDS data analysis can at times become challenging due to the lack of a detailed analytical signal expression or numerical methods with rapid computation time. We have derived the analytical signal expressions κ_{FULL}, for DQC[1] and DEER,[2] including both finite pulse effects and pseudo-secular dipolar coupling, especially important for shorter distances. This framework enables rapid (DQC: 2–6 min; DEER: 1–4 min) and accurate distance reconstructions for both the PDS techniques. In addition to improved accuracy of the data analysis, simulations using κ_{FULL} for DQC demonstrate that the double-quantum filter remains effective even for weak-pulses (14-20 ns π-pulses). This enables DQC experiments on standard commercial spectrometers with low microwave power and without expensive hardware upgrades. We validate the methods on rigid biradicals with known inter-spin distances in the range of about 15 to 32 Å and narrow distributions. The current standard analysis, which uses the simplified signal expressions for DQC and DEER, produces erroneous results for an average inter-spin distance <20 Å. We further applied the weak-pulse DQC, which has a negligible and so an easily

removable background,[3] to flexible polypeptoids and intrinsically disordered tau protein fragments. The improved analysis resolves distinct monomer end-to-end distance distributions for tau wild-type and the disease-associated P301L mutant. Their DQC P(r) differences, previously not distinguishable by DEER, may offer molecular-level insight into their divergent aggregation propensities in neurodegenerative disease. These researches were funded by the NIGMS / NIH under Grant Nos. R24GM146107 and R35GM148272 (ACERT / Cornell), and R35GM136411 (Northwestern).

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ORAL SESSION

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145 Q-band Double Quantum Coherence ESR for Sensitive Nitroxide-based Distance Measurements.

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Recent advances in pulsed dipolar spectroscopy have driven the sensitivity of the technique to physiologically relevant concentrations and extended the applicability to more complex biological systems. The most dramatic improvements in sensitivity have been achieved using orthogonal spin labeling strategies, however, a large majority of ESR applications involves dual nitroxide labels. In our recent breakthrough, we demonstrated Q-band nitroxide double quantum coherence (DQC) ESR for the first time, highlighting deep dipolar modulations of 100% and the ability to resolve multimodal distance distributions. In this work, we further establish DQC at Q-band as a practical technique for distance measurements in doubly nitroxide-labelled proteins. We show that 8 ns ? pulses provide efficient excitation of the double quantum transition at Q-band, though more commonly accessible pulse lengths also yield strong DQC signals. With optimized spectrometer tuning, we achieved signal-to-noise ratios exceeding 100 in just eleven minutes of acquisition for a dipolar evolution time of 1.5 μs for 50 ?M protein samples. We demonstrate the effects of deuteration on sensitivity of the DQC signal, which can further extend dipolar evolution times and the measurable distance range. The DQC results closely match recent theoretical predictions and reveal minimal background contributions from intermolecular interactions, even at concentrations up to 100 ?M. These findings highlight the advantages Q-band DQC for dual nitroxide-labelled proteins, including deep dipolar modulations, low background at micromolar concentrations, and improved sensitivity through deuteration. Collectively, our work positions Q-band nitroxide DQC as a powerful and accessible technique for pulsed ESR distance measurements.

ORAL SESSION

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146 Structural Integrity and Side-Chain Interaction at the Loop Region of the Bridge Helix Modulate Cas9 Substrate Discrimination.

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CRISPR-Cas9 has been revolutionizing genome engineering, and in-depth understanding of mechanisms governing its DNA discrimination is critical for continuing technology advances. An arginine-rich bridge-helix (BH) connecting the nuclease lobe and the recognition lobe, which is conserved across the Cas9 family, exists in a helix-loop-helix conformation in the apo wild-type protein but converts to a long contiguous helix in the Cas9/RNA binary complex. In this work, distances measured with spin labels were utilized to investigate BH's conformational transitions in the solution state upon single-guide-RNA (sgRNA) binding, which is a critical early event preceding DNA binding and cleavage. Analyses show that sgRNA binding drives BH conformational changes in the wild-type SpyCas9 (SpyCas9^{WT}) as well as in two BH-loop variants, SpyCas9^{2Pro} and SpyCas9^{2Ala}. Each Cas9-sgRNA binary complex, however, exhibits distinct BH features that reveal mutation-specific effects on helical integrity vs. side-chain interactions. In addition, the BH conformational variations can be correlated to the observed changes in the mismatch cleavage profiles of the Cas9 variants. The work represents the first use of distances measured by site-directed spin labeling to investigate Cas9 conformational changes in the solution state, and advances our understanding on the structure-dynamic-function relationship governing DNA target discrimination by Cas9.

ORAL SESSION

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147 50 Years of EPR Oximetry from Capillary to Clinic.

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Knowledge of tissue oxygen levels holds paramount importance to understand the mechanism of several pathophysiological disorders and to develop treatment strategies to mitigate disease progression. This would require methods capable of quantifying the level of tissue oxygen with good reliability and accuracy in the clinical setting. Electron paramagnetic resonance (EPR) spectroscopy is capable of measuring tissue oxygen levels using injected (soluble) or implanted (solid) paramagnetic probes as oxygen-sensors. The principle of EPR oximetry is based on the paramagnetic property of molecular oxygen, which can shorten spin-spin relaxation time (T2) of EPR spin-probes leading to EPR line-broadening. The effect of oxygen on EPR spectrum was first observed in DPPH solutions by Deguchi in 1960 and later in nitroxide solutions by others (Edelstein, et. al., 1964; Povich, 1975; Backer, et. al., 1977). The practical application of this phenomenon, termed as 'spin label oximetry', was developed by Hyde and others in the 1980s for studying oxygen transport and metabolism in cell systems. The developments of low-frequency EPR instrumentation and probes during 1990s and later, have enabled the use EPR oximetry for a variety of in vivo applications such as isolated functioning organs (e.g., heart), intact animals, and humans. Over the years, the EPR oximetry technology has continuously evolved, with respect to both the probes and methods, to make reliable, accurate, and repeated measurements in living systems under minimally invasive conditions. The applications of preclinical EPR oximetry are still growing in scope, and include cancer, myocardial infarction, stroke, and wound healing. First studies in clinical oximetry appear promising, with discrete measurement of oxygen using implanted OxyChip probes in cancer patients. This presentation will provide an overview of EPR oximetry, available methods/probes, applications, and some recent advances in the technology for clinical applications.

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ORAL SESSION

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148 Tumor Tissue EPR Oxygen Imaging for Optimizing Interstitial Photodynamic Therapy.

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Interstitial photodynamic therapy (I-PDT) is a promising experimental treatment for patients with locally advanced cancerous tumors that does not respond to the standard-of-care. In I-PDT, light is administered through optical fibers that are inserted into the tumor that activates light sensitive drug (photosensitizer) in the presence of oxygen to produce reactive oxygen species (ROS). After successful demonstration in mouse and rabbit models1, light dosimetry-guided I-PDT has been found safe and potentially effective in a Phase I clinical trial 2 and is being further evaluated in a Phase I/II clinical trial. Our goal in this investigational study was to perform trityl-OXO71-based EPR oxygen imaging during IPDT of locally advanced murine tumors to investigate the effect of tumor oxygenation on the response to I-PDT 3. 10-12 weeks-old female C3H mice with locally advanced SCC7 tumor were treated using a photosensitizer porfimer sodium and the laser (630 nm) with a fluence of 45 J/cm2 and irradiance of either 5.0 mW/cm2 (Cohort 1, n = 7) or 8.4 mW/cm2 (Cohort 2, n = 7) 1, associated with low and high cure rate, respectively 1,2. Another group (n = 7) with no drug and no light was used as a control. The pO2 maps were acquired using a 25 mT/720 MHz instrument, JIVA-25® 4,5. The time to reach the HF10 (Hypoxic fraction below 10 torr) plateau showed a significant difference between the two treatment groups. The average decrease in pO2 in Cohort 1 was smaller than the in Cohort 2, but it was not statistically significant and the change in treatment group was larger than the control group, suggesting that an effective photoreaction does occur at high irradiance of I-PDT. Using high irradiance for delivering the same target fluence (i.e., light dose) optimized using oxygen imaging will reduce treatment time that will be beneficial in clinical settings.

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ORAL SESSION

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149 L-band EPR Spectrometer and Resonators for Rapid Scan.

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Nitroxide radicals are attractive probes for various physiological processes but have shorter relaxation times than trityl radicals. Because of the shorter relaxation times, nitroxides are more amenable to study by rapid scan than by pulse EPR. 1 GHz provides an effective balance between penetration depth and signal-to-noise ratio (S/N) which makes it valuable for rapid-scan EPR preclinical studies. The variable frequency rf source in our rapid scan spectrometer was selected for its low source noise and has a maximum output power of 100 mW. The bridge is designed with the fewest possible components between the resonator and the detector to maximize signal-to-noise. The system's digitizer has advanced time domain firmware, enabling spectra to be averaged directly on the device and effectively eliminating overhead between image projections. Two reflection resonators, an 8 mm loop-gap and a 25 mm saddle coil, were characterized. Gradient coils permit 3D imaging. The number of ^{15}N-nitroxide spins required to achieve a S/N of 3 were 2.0×10^{14} and 4.5×10^{15} for the 8 mm and 25 mm resonators, respectively, with 200,000 averages and a rapid scan frequency of 2.5 kHz. Even with the low-noise source, noise makes substantial contributions at the high powers that give maximum nitroxide signal

amplitude in the larger resonator. Spectra and images that demonstrate performance will be presented.

ORAL SESSION

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150 Trityl OXO71 Distribution Following Intravenous Injection in Rhesus Macaques

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Local tissue oxygen concentration regulation is fundamental to biological processes that govern development, normal physiological function, and pathology. However, only limited experimental methods exist to non-invasively measure pO2 *in vivo*. Electron paramagnetic resonance (EPR) imaging techniques, utilizing the paramagnetic spin probe Trityl OXO71 (referred to as “trityl), possess unique have the capabilities to map pO2 in living organisms. In order to translate previous success utilizing small animal EPR imaging systems to map pO2 in rodent models of human disease, work is underway to develop a large animal EPR imaging system to be used in studies involving nonhuman primates. This presentation will review anticipated applications of trityl-based pO2 imaging in nonhuman primates. It will then present results of pharmacokinetic and distribution studies of trityl following intravenous infusion in three sedated rhesus macaques. Trityl did not perturb physiological parameters such as respiration or pulse rate, supporting the safety of trityl as an imaging agent in translational studies. Plasma concentrations of trityl were observed to be sufficient for pO2 mapping studies for approximately one hour following a bolus intravenous infusion. Ex vivo EPR-based assay of trityl concentration in multiple organs indicate that trityl distribution throughout the body is largely determined by the the blood volume fraction within the sampled tissue, with the exception of the brain in the kidney. In the brain, trityl concentration was negligible, presumably due to limited exchange of trityl across the blood brain barrier. In the kidney, trityl concentration was high due to renal clearance of the compound. Together, these data indicate that EPR imaging of pO2 will be feasible in nonhuman primate subjects following previously-developed strategies adopted in small animal experiments.

ORAL SESSION

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151 Liquid-State DNP at 263 GHz: Advanced Instrumentation to Boost High-Resolution NMR Spectroscopy.

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Overhauser DNP (Oe-DNP) is a powerful technique to enhance NMR signals in liquids. However, Oe-DNP at high fields, relevant for high-resolution NMR spectroscopy, is challenging. Besides reduction of dipolar coupling at higher magnetic fields, which can be compensated with scalar coupling modulated by fast molecular motions[1], high-field DNP still faces difficulties in instrument design since a combination of high-resolution NMR detection with efficient microwave excitation of EPR transitions is needed. Unoptimized microwave excitation on liquid samples leads to low enhancement, heating effects and loss of NMR resolution. Various experimental approaches have been proposed to mitigate these drawbacks, however, a comprehensive solution for all these issues still remains elusive. Here, we present our setup[2,3] in which liquid DNP can be performed close to standard NMR conditions, and with preserved high-field spectral resolution. Thanks to a novel DNP probehead, we achieve hyperpolarization of ^{13}C and ^{19}F in small organic molecules, including essential drugs and natural products, under steady-state conditions in large sample volumes (up to 20 ?L). A sample geometry, spinning and efficient cooling enables suppression of microwave heating. Thus, we demonstrate enhancements up to two orders of magnitude in one- and two-dimensional liquid-state NMR spectra. The developments were facilitated by microwave simulations to access B_1-field strengths and field distributions at the sample position. 263 GHz EPR was applied to gain insight into solvent dependent spectral and relaxation properties of DNP polarizing agents. The setup, the experimental protocols, and particularly the DNP probehead design, will be discussed in detail.

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ORAL SESSION

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152 Pump-induced Dipolar Order to Evaluate Electron Spin Connectivity and Many-body Effects.

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Networks of coupled electrons spins are integral to applications in dynamic nuclear polarization (DNP), quantum information sciences (QIS), and materials properties emerging from many-body correlations. A minimal condition for electron spin entanglement or many-body spin correlations is the presence of dipolar order, where pairs of coupled spins have a preferential alignment – parallel or anti-parallel - across a macroscopic sample. There is a lack of direct experimental techniques to characterize the creation and properties of electron dipolar order across a range of magnetic materials.

In this study, we use off-resonance saturation of the EPR line to initialize pump-induced dipolar order and demonstrate how ELDOR (ELectron DOuble Resonance) and OOP-ESEEM (Out-Of-Phase Electron Spin Echo Envelope Modulation) can be used to probe the formation of dipolar order, with P1 centers in powdered high pressure high temperature (HPHT) diamond samples as our model system. ELDOR experiments on HPHT diamonds show hyperpolarization features that can be attributed to the interconversion of dipolar order to Zeeman order. OOP-ESEEM experiments on these regions which show pump-induced dipolar order generate an out-of-phase signal modulation attributed to dipolar order between P1 centers - to our knowledge the first OOP-ESEEM experiments on pump-initialized dipolar order. Simulations of ELDOR and OOP-ESEEM confirm that the observed experimental signatures could originate from a heterogeneous P1 coupling network.

These results establish new approaches for monitoring the creation and lifetime of dipolar order in systems of coupled electron spins, providing a method for characterizing the potential for spin entanglement and many-body correlation effects in electron spin networks for applications across DNP and QIS.

ORAL SESSION

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153 Coherent Control Over Nuclear Hyperpolarization for Storage Using an Optically Initializable Chromophore-radical System.

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Chromophore radicals (CRs) are emerging as important components in molecular quantum information science (QIS), particularly for quantum sensing applications. In this study, we extend the capabilities of this class of organic materials by exploiting their nuclear spins as highly coherent qubits, thereby providing a platform with significant potential for quantum information storage, computing, sensing, and communication. We demonstrate coherent manipulation of optically initialized electrons in a 1,6,7,12-tetra-(4-tert-butylphenoxy)-perylene-3,4,9,10-bis(dicarboximide) (tpPDI) covalently linked to a partially deuterated 1,3-bis(diphenylene)-d16-2-phenylallyl radical (BDPA-d16) via pulsed Dynamic Nuclear Polarization (DNP) at X-band. Under optical illumination, electron hyperpolarization in BDPA is enhanced 2.4-fold relative to thermal polarization. Using Nuclear Orientation Via Electron Spin-Locking (NOVEL) and reverse NOVEL DNP, we achieve reversible coherent polarization transfer between the optically polarized electron spins and nuclear spins, enabling initialization of predominantly a single localized proton within the CR with a nearly 688-fold enhancement over the thermal polarization of the targeted proton spin and sensitive Electron Paramagnetic Resonance (EPR)-based readout of nuclear spin states. This study allowed us to evaluate the diffusion and relaxation of nuclear spin order, which can help guide the design of next-generation CRs to optimize their performance for QIS or DNP applications. Simulations of nuclear spin diffusion are presented to elucidate the observed nuclear spin relaxation mechanisms. Coupled with CRs robust environmental compatibility, tunability, and precise state initialization - even at elevated temperatures - our results highlight the significant potential of nuclear spins in CRs as a versatile platform for advancing molecular QIS technologies.

ORAL SESSION

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154 Detecting the Effects of Chirality-Induced Spin Selectivity on Electron Donor–Acceptor Molecules.

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The Chirality-Induced Spin Selectivity (CISS) effect is the phenomenon in which electrons obtain a high degree of spin polarization when passing through chiral molecules. Here we use time-resolved electron paramagnetic resonance spectroscopy (TREPR) to show that CISS strongly influences the spin dynamics of photoinduced charge separation in several different covalent donor-chiral bridge-acceptor molecules. Through spectral simulations of the TREPR at X-, Q- and W-band frequencies we can ascertain degree to which CISS contributes to the spin dynamics in randomly oriented powder samples in a frozen glassy solvent at cryogenic temperatures. We show that charge separation through a chiral bridge introduces triplet character into the initial spin state of the radical pair, as opposed to an achiral bridge which results in a radical pair of purely singlet character.

Furthermore, by examining the photoinduced electron transfer in an acceptor-chiral bridge-radical molecule using pulsed EPR measurements, we show that although the spin state of the transferred electron is changed by the CISS effect, its spin entanglement is still maintained.

ORAL SESSION

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155 Photogenerated Spin-Correlated Radical Pairs in Biological, Organic, and Organic-Inorganic Donor-Acceptor Systems.

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Light excitation in organic donor-acceptor systems and natural photosynthetic reaction center proteins (RCs), followed by rapid electron transfer (ET), generates an entangled, magnetically coupled spin pair, known as a spin-correlated radical pair (SCRP) or spin qubit pair (SQP). The SCRP contains detailed information about weak magnetic interactions, structure, and dynamics of local protein environments involved in charge separation processes. However, extracting this information remains a significant challenge.

The high spectral resolution of 130 GHz time-resolved EPR, combined with further enhanced resolution from deuterated proteins, provides new insights into the regulation of light-induced ET. We demonstrated that, in contrast to type II RCs, where ET is unidirectional along one of the two symmetric donor-acceptor ET branches, in type I RCs, such as Photosystem I, both branches are active.

While organic donor-acceptor systems and natural photosynthetic RCs have been widely studied, there are few measurements of photogenerated SCRPs in inorganic systems. Recently, we reported on semiconducting ZnO quantum dots (QDs) connected to organic molecular chromophores. These organic-inorganic hybrid systems, containing highly tailorable QDs, represent a new class of spin-based qubit materials where SQPs can be photogenerated at moderate temperatures. A particular interesting feature of these hybrid systems is that the g-factor of the electron spin in ZnO QDs is outside the range common to organic molecules and can be adjusted due to the quantum size effect in ZnO QDs, which results in higher spin specific addressability than in organic systems, an important requisite of qubit systems.

ORAL SESSION

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156 Observation of Multi-mode Spin-Rabi Oscillation of Strongly EPR Driven Polaron Pairs In a Pi-Conjugated Polymer.

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Electron spin-Rabi oscillations electron paramagnetic-resonantly driven by a linearly polarized, strong radio-frequency domain magnetic field with amplitude B? that exceeds both, the static magnetic Zeeman field B? and the local random hyperfine field difference between polaron pair partners—have been predicted to give rise to long-lived charge carrier spin pair states.[1–3] These states are promising candidates for solid-state qubits due to their anticipated long coherence times and their potential for electrically readable single-spin detection.[4,5] To test the theoretical predictions in,[1] we performed strong-drive pulsed EPR experiments at room temperature using low-field (<0.5mT) pulsed electrically detected magnetic resonance (EDMR). Our measurements focused on spin-dependent polaron recombination currents in OLED devices based on deuterated poly[2-methoxy-5-(2'-ethylhexyloxy)-1,4-phenylenevinylene] (d-MEHPPV), which features reduced hyperfine interactions due to deuteration and thus, well-resolvable EPR peaks at Gauss-domain Zeeman fields. Experiments were conducted in regimes where B? = 0.67 mT, with B? = 0.36 mT (10 MHz) and B? = 0.72 mT (20 MHz). We observed that the integer number N of harmonics found in the Fourier spectrum of the Rabi nutation transient increases linearly with B?, following the relation 4B?/B?, predicted by theory,[1] with harmonics occurring at integer multiples of the drive frequency ?, decaying in a Bessel-function-like manner. Additionally, recombination suppression—a hallmark of strong-drive behavior—was observed over a broad range of B? and ?, in contrast to weak-drive regimes where such effects are confined near the on-resonance condition only.

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ORAL SESSION

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157 Quintet-to-Radical Spin Polarization Transfer in Pentacene–Radical Hybrid Polymers.

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Spin polarization transfer from photoexcited states to stable radicals is an important pathway/tool for advancing quantum sensing. While triplet to radical polarization transfer is well studied, often utilizing radicals like BDPA and trityl, polarization transfer from quintet multiexciton states, arising from singlet fission (SF), remains largely unexplored.

Quintet states, characteristic of efficient SF, offer unique polarization patterns and long spin lifetimes, making them attractive for spin storage and transduction. Here, we investigate a series of pentacene pendent polymers with covalently bound BDPA radicals to elucidate quintet-to-radical polarization transfer. These polymeric materials combine efficient SF and tunable radical spacing within a modular, solution-processable scaffold.

Using transient EPR spectroscopy, we track the dynamics of spin-polarized intermediates and identify spectral features consistent with quintet-to-radical transfer. These findings reveal new spin transport mechanisms in SF-based hybrids and broaden the role of multiexcitonic states in molecular quantum technologies.

ORAL SESSION

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158 Structural Contributions to Spin-Exchange Interactions and Spin Polarization in Pentacene-Radical Dyads.

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The role of spin coupling interactions on the photophysical properties of open shell molecular systems is of interest in the development of magnetic resonance and quantum sensing methods. The strength of the magnetic exchange interaction between spin systems can define the outcome of the photophysical pathway and ultimately the state of the system following optical irradiation.

Using multireference methods[1] we study the structural contributions to the magnitude and sign of the magnetic exchange interaction, J_{TR}, between a pentacene triplet and a radical doublet. The magnitude and sign of J_{TR} is highly dependent on the extent of conjugation and position of the bridge linking the pentacene and radical moieties. Our results provide an intuitive picture using spin density maps for how to tune these interactions in pentacene radicals. We calculate the exchange interactions between more than 30+ different pentacene-radical structures using 3 different radicals including the wide-line TEMPO and narrow-line trityl and BDPA radicals. In addition, we extract interconversion (IC) rates from calculated J_{TR} parameters and energies.

We also investigated the transient absorption and transient electron paramagnetic resonance (trEPR) spectra of pentacene nitroxide radicals having varying degrees of ferromagnetic coupling. We observe a decrease in the singlet lifetime of pentacene in 3 species but no evidence of intersystem crossing. To investigate the coupling between the two moieties we use trEPR in combination with an anthracene sensitizer to populate the pentacene triplet. Under these conditions we observe polarization of the nitroxide radical in the species exhibiting large positive ferromagnetic coupling.

In this presentation we will describe our current understanding of the mechanisms of the nitroxide polarization and efforts towards designing systems exhibiting favorable kinetics for generating large ground state spin polarization in organic radicals. Based on calculated IC rates among the 30+ different pentacene-radical structures and comparisons with previously published data, we propose structural motifs that optimize interconversion rates in pentacene-radical systems.

ORAL SESSION

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200 Broadband and Selective Inversion of Electron Spins at Q-band Frequencies.

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Recently, microwave pulse shaping has become a valuable tool for enhancing sensitivity of EPR spectroscopy and expanding its scope towards novel applications. From the perspective of structural biology, pulsed EPR dipolar spectroscopy, particularly Double Electron Electron Resonance (DEER, aka PELDOR)[1] and Single Frequency Technique for Refocusing Dipolar Couplings (SIFTER)[2] techniques, have benefited from enhanced excitation profiles provided by the shaped pulses.[3-7] On the other hand, novel EPR application avenues, such as quantum information science and spin-based quantum technologies require not only broadband excitation, but also ability to manipulate electron spin ensembles with high fidelity as well as preparation, control and read-out of the specific states of a quantum system. EPR application scope ranging from structural biology to spin-based quantum technologies that can be addressed by a single experimental platform needs a flexible, yet accurately controllable experimental architecture. As such, we developed microwave resonators with high uniformity of B_1, where B_1-bandwidth is adjustable in accurate manner. Moreover, we integrated arbitrary waveform generator using a concept of intermediate frequency (IF) that enabled efficient control of pulse excitation bandwidth, pulse shape and its resonance position in EPR spectra. Utilizing a Q-band loop-gap resonator with the excitation bandwidth of exceeding of 600 MHz and FT-EPR experiment architecture, we demonstrated broadband and selective inversion of electron spin sub-ensembles coupled to nitrogen nuclei with a specific spin state using a diamond powder sample.

1. Pannier et al, *J. Magn. Reson.*, **2000**, *142*, 331.

2. Jeschke et al, *Chem. Phys. Lett.*, **2000**, *331*, 243.

3. Doll et al, *Phys. Chem. Chem. Phys.*, **2016**, *18*, 23111.

4. Spindler et al, *Angew. Chem.*, **2013**, *52*, 3425.

5. Endeward et al, *J. Magn. Reson.*, **2023**, *136-137*, 61.

6. Schöps et al, *J. Magn. Reson.*, **2015**, *250*, 55.

7. Doll et al, *J. Magn. Reson.*, **2013**, *230*, 27.

POSTER SESSION

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201 Development of Rapid-Scan EPR Spectrometer and Imager at L-band (1.0 GHz).

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In rapid-scan EPR the main magnetic field is constant and auxiliary coils are used to scan the magnetic field at kHz rates. For many types of radicals the rapid scans result in improved signal-to-noise per unit time.[1] The signal is detected in quadrature and software is used to convert the time trace to a magnetic-field axis and restore the slow-scan absorption spectrum. The rapid magnetic field scans create an oscillating background signal. Separation of the EPR signal from the background signal is done in software. The use of the Matlab routine backcor in background corrections will be discussed. Unlike pulsed EPR, the rf source is on during signal detection which means that selection of the rf source with the lowest noise, especially at higher powers, is important to maximizing system performance. This was the basis for selection of the Rohde & Schwartz SMA100B. Source noise is a substantial issue for the larger resonators required for in vivo studies because larger resonators have lower efficiency, $B_1/\sqrt{W}$ where W is the incident power. Resonator efficiency was measured by comparing power saturation with that in resonators that have known efficiency and by the method of perturbing spheres. The rapidly scanned field also may cause microphonics that are resonator dependent, which adds noise in the spectra. Signal-to-noise was compared for aqueous solutions of nitroxide radicals in two volume resonators – a loop gap resonator for 8 mm tubes and an Alderman-Grant resonator for 25 mm tubes and for surface coil resonators with 10 mm or 30 mm diameters. The number of ^{15}N-nitroxide spins required to achieve a S/N of 3 was 2.0×10^{14} (8 mm resonator), 4.5×10^{15} (25 mm resonator), 2.7×10^{14} (10 mm surface coil) or 1.4×10^{16} (30 mm surface coil). For the volume resonators the solution filled the resonator and for the surface coils the samples were in 1 mm thick plates directly above the coil. Spectra were acquired with 200,000 averages and a rapid scan frequency of 2.5 kHz.

(1) Eaton, G. R.; Eaton, S. S. Rapid Scan Electron Paramagnetic Resonance. In *EPR Spectroscopy: Fundamentals and Methods*, Goldfarb, D., Stoll, S. Eds.; John Wiley & Sons, 2018; pp 503 - 520.

POSTER SESSION

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202 Multifrequency Study of Multiphoton Electron Paramagnetic Resonances in Crystalline $Gd^{3+}:YVO_4$

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The lanthanide ion gadolinium doped in crystalline yttrium orthovanadate ($Gd^{3+}:YVO_4$) is an air-stable, spin S = 7/2 paramagnet with magnetic field-tunable spin energy levels due to its crystal field interactions. These properties make it a promising test ground for multilevel quantum state (*qudit*) operations via electron paramagnetic resonance (EPR) spectroscopy. In particular, its high spin and tunable anharmonicity favor the implementation of multiphoton state initialization, as proposed by Lauenberger and Loss.[1] As a first step toward this end, we have conducted multifrequency EPR studies of $Gd^{3+}:YVO_4$ in order to identify multiphoton resonances experimentally and compare their signatures to theoretical predictions.

1. M. Leuenberger and D. Loss, *Nature* **410**, 789 (2001).

POSTER SESSION

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203 Electronic Wavefunction Delocalization Beyond the Metallic Core of Palladium Dodecanethiolate Nanoparticles: Revealed through Pulse ESR.

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1. The Pennsylvania State University, Department of Chemistry, University Park, PA 16802

Ligand-stabilized metallic nanoparticles exhibit diverse functionality across catalysis, sensing, and biomedicine driven by the behavior of itinerant electrons. The electrons delocalized nature give rise to the most desirable properties of nanoparticles such as their conductivity, high density of states, and enhanced polarizability. These attributes are often conceived as characteristics of the core which is distinct from the ligand and solvent shells. However, there is scant research exploring the extent of the metallic core wavefunction delocalization into the surrounding chemical environment. The electron and nuclear spin couplings of palladium dodecanethiolate nanoparticles has been discovered through pulse electron spin resonance. Systematic exploration of labeled and unlabeled ligands and solvent demonstrated that both nuclear spins from the thiol and solvent were coupled to the electron spin of the metallic core. Thus revealing the metallic electrons are not isolated to the core, but rather extend through-space interactions. These preliminary results serve as a basis to begin further investigation into directed tunability of the metallic wavefunction propagation for controlled functionality.

POSTER SESSION

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204 Optomechanical Phase Shifters for Free-electron-laser Powered Agile Pulsed Electron Spin Resonance Spectroscopy.

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1. Physics Department and Institute for Terahertz Science and Technology, University of California, Santa Barbara, California, 93106

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For studies of spin relaxation times in many systems—for example, molecules with large zero-field splittings, or fermionic collective excitations in quantum magnets—it is highly desirable to perform pulsed ESR experiments at high magnetic fields with sufficiently high power to resolve ns relaxation times while operating over a wide range of frequencies above 100 GHz. At UCSB, a unique free-electron-laser-powered agile pulsed ESR (FELAESR) spectrometer is nearing completion. The FELAESR spectrometer is designed to measure ns spin

relaxation times at magnetic fields up to 16 T at frequencies tunable between 170 and 420 GHz and temperatures of ~2 to 300K. This poster will describe the design and implementation of software-controlled, frequency-agile, mechanical phase shifters used in conjunction with complementary channel pulse slicers[1] in a bar configuration as a complete pulse forming module. This device enables phase cycling by introducing a controlled phase shift to an incident Gaussian beam by physically extending the optical path length via a precision-aligned trio of mirrors mounted on a motorized sliding platform. Unlike fixed-frequency phase cycling methods,[2] our phase shifter operates effectively across the full tuning range of our FEL, enabling robust phase cycling in frequency-sensitive EPR studies. The system achieves a step resolution of 51.7±0.5 ?m per motor increment, allowing for fine control over phase shifts—0.04 degrees per step for 240 GHz—with high reproducibility. Two of these phase shifters are used alongside three complementary-channel pulse slicers to convert a single FEL pulse into three pulses with independently-tunable duration and relative phase. The insertion loss of the two phase shifter modules in the bar assembly is less than 1 dB. The phase shifters and pulse slicers could also be used to convert the cw output of gyrotrons into sequences useful for high-field pulsed ESR.   This work was supported by NSF-DMR 2117994.

(1) Price, B. D.; Sojka, A.; Agladze, N. I.; Sherwin, M. S. Compact module for complementary-channel THz pulse slicing. *Applied Physics Letters* **2024**, *124* (2). DOI: Artn 021107 10.1063/5.0180412.

(2) Wilson, C. B.; Aronson, S.; Clayton, J. A.; Glaser, S. J.; Han, S. G.; Sherwin, M. S. Multi-step phase-cycling in a free-electron laser-powered pulsed electron paramagnetic resonance spectrometer. *Phys Chem Chem Phys* **2018**, *20* (26), 18097-18109. DOI: 10.1039/c8cp01876f.

POSTER SESSION

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205 Quintet-to-Radical Spin Polarization Transfer in Pentacene–Radical Hybrid Polymers.

Jasleen K. Bindra,[1] Daniel Malinowski,[2] Bernardo Salcido-Santa Cruz,[3] Guiying He,[4] Matthew Y. Sfeir,[3,4] Luis M. Campos,[2] Jens Niklas,[1] Oleg G. Poluektov[1]

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Spin polarization transfer from photoexcited states to stable radicals is an important pathway/tool for advancing quantum sensing. While triplet to radical polarization transfer is well studied, often utilizing radicals like BDPA and trityl, polarization transfer from quintet multiexciton states, arising from singlet fission (SF), remains largely unexplored.

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Using transient EPR spectroscopy, we track the dynamics of spin-polarized intermediates and identify spectral features consistent with quintet-to-radical transfer. These findings reveal new spin transport mechanisms in SF-based hybrids and broaden the role of multiexcitonic states in molecular quantum technologies.

POSTER SESSION

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206 EPR Characterization of Molten Salt Synthesized Erbium(III) Doped Yttria Nanoparticles.

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Molten-salt synthesized Er^{3+}:Y2O3 nanocrystals is a promising platform for quantum sensing due to desirable optical and magnetic properties. Through X-band CW-EPR experiments the Er^{3+} spin centers are shown to retain a spectrum consistent with systems along with the presence of Y_2O_3 crystal defect centers and impurities.[1] Pulsed EPR experiments were performed to determine relaxation properties and mechanisms including T_1 and T_m anisotropy, instantaneous diffusion, spectral diffusion, and temperature-dependent spin–lattice relaxation. Instantaneous diffusion measurements show a small impact on T_m. Temperature-dependent T_1 and T_m measurements from 4-7 K are consistent with a Raman process and electron-electron spectral diffusion.[2]

1. T. Rajh et al., Mater.Quantum.Technol., 2022, 2, 045002

2. X. Du and L. Sun, Inorg. Chem. Front., 2024, 11, 8660-8670

POSTER SESSION

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207 An EDMR and NZFMR Study of Defects Generated in SiO_2 by High Electric Field Gate Stress.

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Time dependent dielectric breakdown (TDDB) is a fundamental failure mechanism in semiconductor devices where a conductive path is generated through a dielectric material by a high electric field. This phenomenon is most important in metal oxide semiconductor field e@ect transistors (MOSFETs) the primary building block of modern solid-state electronics. There is little atomic-level understanding of how a conductive path develops through a MOSFET gate dielectric from high electric fields. We use electrically detected magnetic resonance (EDMR) and near zero-field magnetoresistance (NZFMR), with an electrical characterization technique—direct current IV (DCIV) measurements—to investigate the high electric field gate stress phenomena. We performed two studies: one involved long-term stress using NZFMR at time intervals from zero to two thousand minutes of gate stress, another repeating the process using EDMR during the early stress phases to identify the defects present as TDDB progresses in SiO2. N-MOSFETs with 7nm SiO2 gate oxides were pre-characterized using the magnetic resonance and electrical characterization techniques, then stressed at 7.5V, and the same measurements were repeated. Long-term positive gate electric field stress generates an initial jump in interface traps detected via DCIV current and the NZFMR response, which levels out after 10 minutes of stress. As the stress time continues, the number of interface traps does not rise, but the location of the DCIV peak shifts due to the buildup of bulk charges. Negative gate bias stress generates a steady increase in interface traps at a lower magnitude than positive stress with no change in DCIV peak location. EDMR measurements were utilized for preliminary defect identification. The EDMR results suggest the generation of two defects with zero crossing g values of about 2.0068 and 2.0006, consistent with Pb and E' centers.

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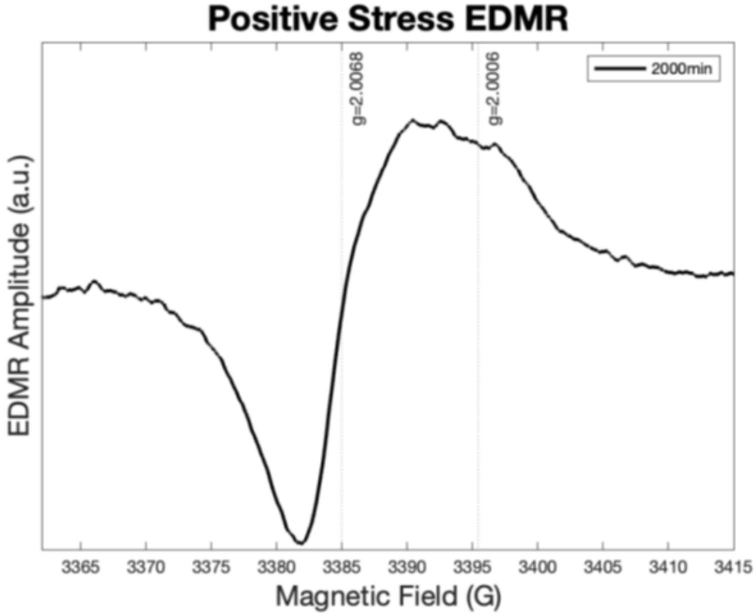

Post-stressing EDMR spectrum of a MOSFET suggesting generation of both interface and oxide trapping centers

POSTER SESSION

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208 Near Zero Field Magnetoresistance and Electrically Detected Magnetic Resonance Investigation of 4H-SiC PN Junctions.

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We have made Near Zero Field Magnetoresistance (NZFMR) and Electrically Detected Magnetic Resonance (EDMR) Measurements as a function of forward bias voltage and modulation frequency. All measurements were made at room temperature and involve NZFMR amplitude and lineshape as a function of forward bias voltage and modulation frequency. Our primary interest in this investigation is evaluating the potential of these devices for utility in quantum magnetometers[1]. We find that the response is a strong function of both junction forward bias voltage and modulation frequency. The NZFMR quantum magnetometers will be most effective if they primarily utilize a very sharp feature. This sharp feature is a very strong function of the forward bias voltage and more weakly dependent upon the modulation frequency. We have made parallel measurements on these devices utilizing low-field EDMR. A combination of NZFMR and EDMR may be useful in self-calibration of the magnetometers. Although space limitations do not allow for detailed discussion, it is clear that the optimization of 4H-SiC PN junctions will involve both materials chemistry and device geometry. To the extent that it is possible, we will discuss these features in our poster presentation should it be accepted for the Rocky Mountain Conference on Magnetic Resonance.

1. C. J. Cochrane, J. Blacksberg, M. A. Anders, and P. M. Lenahan, *Scientific Reports*, 6, (1), 37077, (2016).

POSTER SESSION

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209 Flavoproteins as Native and Genetically Encoded Spin Probes for in Cell ESR Spectroscopy.

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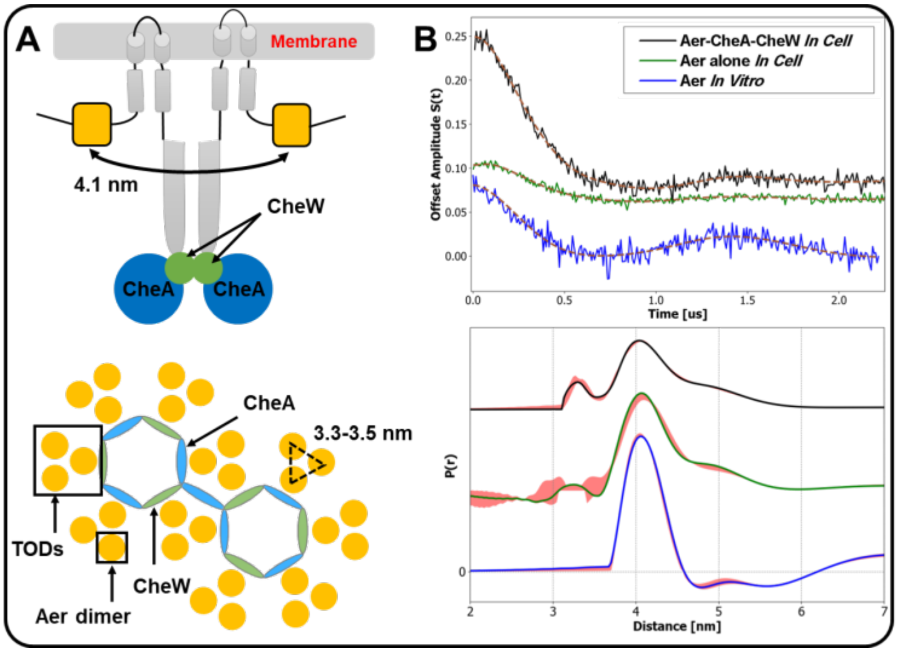
The use of spin probes has been limited by their permeability and their chemical stability in cell. To overcome this challenge, we developed a new category of spin labels that are based on flavoproteins. We studied the transmembrane receptor Aer as a model system containing stable flavin radicals *in vivo* and we elaborate a genetically encoded flavoprotein domain iLOV as a spin label that could be expressed genetically and attached directly *Escherichia coli* (*E. coli*) to a protein of interest.

Most mobile bacteria move towards favorable environments by exhibiting a behavior known as chemotaxis[1]. In *E. coli*, Aer is a primary energy sensor for mobility. Aer responses are determined by the redox state of the flavin adenine dinucleotide (FAD) cofactor, which sends signals from the electron-transport chain to the chemotaxis histidine kinase CheA[2]. Aer has been previously studied by electron spin resonance (ESR) in reconstituted systems with membranes or nanodiscs[3]; however, such systems do not recapitulate the higher-order assembly states chemoreceptors that Aer likely form to amplify signals.

In this study, we optimize biochemical and spectroscopic conditions to investigate Aer and obtain insight by 4P-DEER on the organization of Aer in chemosensory arrays. In parallel, we bioengineer a flavoprotein domain iLOV and fuse it to CheA, revealing domain associations that only occur *in vivo*. Whole cell isotopic labeling (^2H or ^{15}N) is also carried out to improve the distance range measurement obtained by 4P-DEER and to achieve the complete characterization of the spin system by cw-ESR and hyperfine pulsed ESR spectroscopy. These live-cell studies have the potential to reveal signaling features of proteins involved in chemotaxis. This research has been submitted to Nature Communication[4] and is supported by Supported by NIH R35GM122535 (BRC) and NIH R35GM148272 (JHF) and R24GM146107, P41GM103521 (JHF & BRC).



1. B.L. Taylor et al.; *Annu. Rev. Microbiol.*, **1999**, 53, 103–128.
2. Z.A. Maschmann, et al.; *J. Biol. Chem.*, **2022**, 298, 102598.
3. D. Samanta, et al.; *J. Biol. Chem.*, **2016,** 291, 25809-25814
4. T. Chauviré, et al., *Biorxiv* **2024**, https://doi.org/10.1101/2024.12.18.628722

POSTER SESSION

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210 Measurement of TEMPO Reduction to Determine Storage Effects on Antioxidant Levels in Fruits and Vegetables II.

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Insufficient antioxidant levels in the human body can lead to oxidative stress, which can contribute to Alzheimer's disease, obesity, poor health-related quality-of-life, and other issues.[1, 2] Our experiment uses EPR (Electron Paramagnetic Resonance) to measure the reduction rate of TEMPO (2,2,6,6-tetramethylpiperidine-N-oxyl) with various fruits and vegetables as a measure of antioxidant activity.[3] Detailed results from a variety of different produce items were obtained, and any differences in antioxidant capacity among different storage methods (e.g., frozen versus fresh) were noted. First-order rate constant values (s^{-1}) ranged from $k = 1.40 \times 10^{-5}$ to 7.66×10^{-3}. To distinguish major variations in the reduction rates of TEMPO by the different samples, we divided the rates into three groups: fast ($k > 1.00 \times 10^{-3}$), medium ($k = 1.00 \times 10^{-4}$ to 1.00×10^{-3}), and slow ($k < 1.00 \times 10^{-4}$). Garlic reduced TEMPO the fastest ($k = 7.66 \times 10^{-3}$); blueberry and blackberry were the slowest ($k = 3.88 \times 10^{-5}$ and 1.40×10^{-5}), which was surprising given the advertising emphasis on their antioxidant capacity. Some samples (garlic, strawberry, and cilantro) showed biphasic TEMPO reduction rates, suggesting multiple antioxidant species. We conclude that while there was little difference in antioxidant activity across differently stored samples of the same produce item, fresh-picked produce typically showed faster reduction rates than their store-bought or frozen equivalents.

1. Wu et al., *J. Cardiovasc. Nurs.,* **2023**, 38, 6.

2. Reddy, *Biomedicines,* **2023**, 11, 2925.

3. Cheng and Morse, **2024**, RMCMR 63:215.

POSTER SESSION

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211 Probing Alternating Exchange Interactions in a Molecular Spin Chain via HFEPR.

Lima L.G[1]., Havlícek L.[1], Arenas D.[1], Sartoris, R.P[2]. and Santana V.T[1].

[1] Central European Institute of Technology, Brno University of Technology, Brno, 61200, CZ.

[2] Departamento de Física, Facultad de Bioquímica y Ciencias Biológicas, Universidad Nacional del Litoral (UNL), 3000 Santa Fe, Argentina.

Molecular materials that feature spin chains with alternating exchange interactions serve as experimental realizations of low-dimensional magnetic systems, ideal for investigating quantum correlations and collective spin dynamics.[1] These materials, such as transition metal coordination compounds can have spins arranged along a chain, where magnetic interactions can occur through chemical pathways between neighboring sites either via covalent bonds, ?-? stacking or hydrogen bonds.[1] These types of arrangements can result in competing ferromagnetic or antiferromagnetic couplings, which can be measured by spectroscopy techniques.[2] This study focuses on synthesis and characterization of $[Cu_2(\mu\text{-}OH_2)_2L(phen)_2(NO_3)_2]$ (phen=phenanthroline, L=fumaric acid) using high-frequency electron paramagnetic resonance (HFEPR) between 90 GHz and 480 GHz and magnetic field up to 16 T in powder and single-crystals samples between 3 K and 300 K and DC magnetic susceptibility measurements. The intramolecular interaction is equatorial supported by an aqua bridge Cu-O-Cu with an angle of 99.7° and a distance of 3.58 Å. There are two pathways for the intermolecular exchange, one via equatorial-equatorial covalent bonds through L with 10.7 Å and another equatorial-apical via hydrogen bond with 7.1 Å. Ghoshal et al. reported susceptibility data for a similar compound with L = succinic acid, resulting in an intramolecular antiferromagnetic coupling $J = -2.74\ cm^{-1}$ and an intermolecular ferromagnetic coupling $J' = 0.10\ cm^{-1}$.[3] In our system, we observed changes in the EPR spectra below 50 K, with a shift of the parallel and perpendicular g-factors in agreement with a model of weakly coupled

S = 1 chains using a nearest-neighbor uniaxial Heisenberg chain model, providing a ferromagnetic coupling J' = 0.06 cm^{-1}.[4] At last, we will discuss the observed EPR spectral features that would be inaccessible at low probing frequencies, enabling the analysis of anisotropies, the g-matrix, dipolar and exchange spin-spin interactions between the coupled centers.

1. A. Fainstein et al., J. Phys.: Condens. Matter 4, 4989 (1992)
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3. D. Ghoshal et al., Dalton Trans, 1687 (2004)
4. I. Jakovac et al, Phys. Rev. B 111, 064407 (2025)

POSTER SESSION

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212 Advances in Distance Measurement Throughput and Sensitivity through a Superconducting Resonator Platform.

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Pulsed Dipolar Spectroscopy (PDS), a branch of Electron Paramagnetic Resonance (EPR) spectroscopy focused on the measurement of nanoscale electron-electron distances via the strength of their dipolar interaction, has garnered significant interest within the scientific community in recent decades. PDS can provide rich structural and dynamic information on biomolecules that may be difficult or impossible to attain through alternative biophysical methods such as Cryo-EM, NMR, and X-ray crystallography, making it an attractive technique in the field of structural biology at large. However, PDS faces obstacles to its widespread adoption into standard structural biology workflows, such as the steep learning curve to conducting distance measurements and low sample throughput. Here, we present advancements in distance measurement methodology and system automation, leading to higher measurement sensitivity and sample throughput.

These enhancements are enabled by a compact superconducting resonator device, enabling high stability and micromolar sensitivity with small sample volumes and a compact form factor. The stability and sensitivity of the instrument allow for long, uninterrupted data collection with no phase drift, for unattended sequential acquisitions. Such stability is also ideal for advanced distance measurement methods such as DEER-Stitch, RELOAD, and CPMG pulse trains, which can greatly enhance measurement sensitivity. Furthermore, high throughput is facilitated by the automation of sample handling, sample characterization, data collection, and distance analysis. Finally, we exhibit multisample capabilities, with up to five samples being introduced into the cryostat simultaneously for multiple sequential data acquisitions with no input necessary between samples. The work presented here represents important progress in broadening the accessibility and application of EPR into diverse scientific disciplines.

POSTER SESSION

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High-Power 263 GHz Pulsed-EPR Spectrometer for the Elucidation of Transition Metals in Protein Systems.

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Advanced Pulsed-Electron Paramagnetic Resonance (EPR) studies of transition metals in biological complexes at high frequencies demand stringent requirements. First, the sample space must be manageable for users to load in their solution with sufficient spins, which can be difficult with typical resonators at high frequencies. Second, the pulses should be sufficiently short to enable reasonable excitation of the spins, which requires significant microwave power. Here, we develop a quasi-optical[1] 263 GHz pulsed-EPR spectrometer equipped with a non-resonant cavity and a world-unique 10 W-Travelling Wave Tube (TWT) amplifier[2]. The cavity enables us to load samples up to ~10-12 uL, comparable to volumes at Q-band. Additionally, the 10 W TWT amplifier enables a pi-pulse of 60 ns. Furthermore, the TWT has a 10-GHz bandwidth, ensuring the capabilities of multi-frequency advanced pulsed techniques. Overall, the high-powered 263 GHz pulsed-EPR spectrometer opens the avenue for elucidating transition metals in various biological and medical contexts. Supported by NIH 1R35GM126961.

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POSTER SESSION

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214 Antioxidant Loaded Beta-Cyclodextrin Nanofibers for Preventing Edible Oil Degradation.

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Cyclodextrins (CDs) are cyclic oligomers of glucose linked via ?-(1,4) glycosidic bonds, resulting in a distinctive truncated cone structure. Their hydrophobic cavity enables the formation of guest–host complexes with a wide range of organic compounds, and the size of this cavity grows with the number of glucose units—?-CDs containing 6, ?-CDs 7, and ?-CDs 8 monomers, respectively. This study investigates pullulan-CD nanofiber membranes loaded with tocopherol to prevent oxidative degradation in edible oils through controlled antioxidant release. To study this system, we use Electron Spin Resonance (ESR) spectroscopy, a uniquely suitable technique that directly measures antioxidant activity by detecting changes in free radical concentrations. We first simulate accelerated oil degradation conditions, such as heating and UV exposure, to evaluate the protective effect of the antioxidant loaded pullulan-CD membranes. We developed a stop-flow ESR system to ensure precise mixing of tocopherol-loaded nanofibers with the stable radical DPPH (2,2-diphenyl-1-picrylhydrazyl) allowing real-time monitoring of the decrease in DPPH concentration. The kinetics of this reaction reveal the tocopherol release rate from the CD cavity into the solution, which we aim to optimize for practical food industry applications. Additionally, heat-stress testing ESR experiments were performed on various edible oils including sunflower, Sacha inchi and grapeseed oil. The formation of free radicals under heat stress is monitored by spin trapping with PBN (N-tert-Butyl-?-phenylnitrone). Comparing ESR signal changes across various oil samples containing different CD fiber/tocopherol compositions provides insight into their effectiveness as controlled-release systems to slow oxidative spoilage. Through ESR-based monitoring of antioxidant release kinetics under stress, this work develops efficient pullulan-CD nanofiber membranes as advanced antioxidant delivery platforms for oil preservation.

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POSTER SESSION

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215 In-cell Cu(II)-NTA Labeling for EPR Distance Measurements.

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To gain an holistic understanding of protein function, structure and dynamics measurements must be carried out in-cell to account for molecular and physical crowding effects. Recent developments in EPR methodology have revealed the power of this technique to measure structural constraints in-cell. However, there remains a serious bottleneck, as proteins must be labeled ex-situ or using noncanonical amino acids. In this work, we expand current endogenous labeling methods using the Cu(II)-NTA spin label, quantify the amount of spin label delivered into the cells, assess spin labeling, and account for orientational effects during distance measurements.1 Additionally, we show that hypotonic swelling is a reliable method deliver Cu(II)-NTA into cells, achieving a bulk average of 57uM spin labeled site across six repeats. Our work provides a way to circumvent the current endogenous labeling bottleneck, making in-cell spin labeling accessible to the broader EPR community.

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POSTER SESSION

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216 Optically Detected Magnetic Resonance Spectroscopy of Carbon and Nitrogen in Soil and Plant Analytes Using a Microfluidic Diamond Quantum Sensing Platform.

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Agriculture is essential for the growth of every country in terms of food security, but at the same time, agriculture also significantly contributes to greenhouse gas emissions—for instance, large water consumption and excessive fertilizer use present substantial environmental challenges. To promote sustainable agriculture, it is critical to minimize carbon (C) and nitrogen (N) losses while ensuring optimal production levels.[1] However, a major challenge is the accurate measurement of soil nitrate concentrations, which is crucial for effective crop management and environmental protection. We aim to develop chemical sensors based on an integrated microfluidic-diamond quantum sensing platform to address these issues.[2] Nitrogen vacancy (NV) centers offer exceptional magnetic sensitivity (~0.75 nT Hz?$^{1/2}$) and spectral resolution (~0.65 Hz), allowing detection of ^{13}C and ^{14}N spins in pico-liter volumes.[3] This approach overcomes key limitations of conventional inductive Electron paramagnetic resonance (EPR)/nuclear magnetic resonance (NMR) spectrometers, including low sensitivity with longer and susceptibility to soil-derived magnetic artifacts. First, we show results on optimizing the diamond substrates with longer coherence lifetimes (T?/T?) by using optically detected magnetic resonance (ODMR) and XY-8 correlation spectroscopy[4,5] to detect ^{1}H protons and ^{19}F nuclear spins in oils. Then, we show the design and fabrication steps of a microfluidic device that enhances the proximity of NV sensing of ^{14}N in nitrates from soil/plant samples. The successful implementation of this technology will provide real-time, in-situ monitoring of key soil and plant nutrients, facilitating data-driven agricultural decisions. The outcomes of this project could significantly advance precision agriculture, ultimately supporting food security and ecological sustainability. Supported by The National Science Foundation Award 2426522 and the University of Nebraska-Lincoln Grand Challenges catalyst award entitled “Quantum Approaches addressing Global Threats.

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POSTER SESSION

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217 Development of Hardware and Protocols for Ex-Vivo Rat Liver Oxygen Imaging.

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Orthotopic organ transplantation remains the only viable method for treating end-stage organ diseases, however,

current preservation times for whole organs are limited to only a few hours of storage, which results in wastage

of critical organs.1-3 Organ preservation is a multi-step process that is potentially damaging to the organ and the noninvasive assessment for viability and function is important to optimize the preservation methods and increase the storage time. Trityl-based EPR oxygen imaging is the only method that provides partial oxygen pressure (pO2) maps that can be used to assess the cell and organ viability 4,5. In this study, our goal was to develop and optimize hardware and protocols for ex-vivo rat liver oxygen imaging. We designed and built a horizontal rectangular resonator of 60x60x30 mm dimensions for JIVA-25®, one of the largest resonators ever developed for an EPROI instrument, which could accommodate a 60 mm diameter petri dish containing a rat liver. We optimized image acquisition parameters and compared three trityl delivery methods to livers: (i) passive soaking of the liver in trityl, (ii) manual injection of trityl via portal vein cannulation, and (iii) controlled perfusion of oxygenated trityl to the liver. All three delivery methods successfully enabled the acquisition of multiple pO_2 maps with clear vascular features, and portal vein branches. Although imaging during perfusion with oxygenated trityl was more challenging, this was mitigated using a deep learning-based denoising algorithm 6. This work demonstrates the feasibility of high-resolution pO2 mapping of ex vivo rat livers. These results lay the foundation for future EPROI studies in larger organs and highlight EPROI's potential for assessing organ viability.

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POSTER SESSION

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218 Coherent Control Over Nuclear Hyperpolarization for Storage Using an Optically Initializable Chromophore-radical System.

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Chromophore radicals (CRs) are emerging as important components in molecular quantum information science (QIS), particularly for quantum sensing applications. In this study, we extend the capabilities of this class of organic materials by exploiting their nuclear spins as highly coherent qubits, thereby providing a platform with significant potential for quantum information storage, computing, sensing, and communication. We demonstrate coherent manipulation of optically initialized electrons in a 1,6,7,12-tetra-(4-tert-butylphenoxy)-perylene-3,4,9,10-bis(dicarboximide) (tpPDI) covalently linked to a partially deuterated 1,3-bis(diphenylene)-d16-2-phenylallyl radical (BDPA-d16) via pulsed Dynamic Nuclear Polarization (DNP) at X-band. Under optical illumination, electron hyperpolarization in BDPA is enhanced 2.4-fold relative to thermal polarization. Using Nuclear Orientation Via Electron Spin-Locking (NOVEL) and reverse NOVEL DNP, we achieve reversible coherent polarization transfer between the optically polarized electron spins and nuclear spins, enabling initialization of predominantly a single localized proton within the CR with a nearly 688-fold enhancement over the thermal polarization of the targeted proton spin and sensitive Electron Paramagnetic Resonance (EPR)-based readout of nuclear spin states. This study allowed us to evaluate the diffusion and relaxation of nuclear spin order, which can help guide the design of next-generation CRs to optimize their performance for QIS or DNP applications. Simulations of nuclear spin diffusion are presented to elucidate the observed nuclear spin relaxation mechanisms. Coupled with CRs robust environmental compatibility, tunability, and precise state initialization - even at elevated temperatures - our results highlight the significant potential of nuclear spins in CRs as a versatile platform for advancing molecular QIS technologies.

POSTER SESSION

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219 Two-Axis Rotating Sample Holder for Cryogenic, High Field EPR.

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We present the design and implementation of a software-controlled two-axis rotating sample holder for use in various cryogenic, high-field electron paramagnetic resonance (EPR) experiments. This device is constructed with EPR-silent materials and can operate at temperatures as low as 1.6K and magnetic fields up to 16T. Unlike conventional rotating sample holders which mainly utilize gear-based mechanisms, this sample holder features a piezoelectric motor (attocube ANR51/RES/LT/HV), which eliminates kickback and enables precise orientation-selective EPR even at cryogenic temperatures. The device has demonstrated a precision of ~50m° at room temperature and ~0.1° under cryogenic, high field settings wtih high reproducibility. This device serves as the cornerstone for an ongoing study regarding Cu(L-Met)$_2$—an organometallic complex whose Cu^{2+} ions form a spin array that give rise to strongly anisotropic EPR signals. This work was supported by the National Science Foundation under Grant No. NSF-DMR-2117994.

POSTER SESSION

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220 Probing Fundamental Magneto-Structural Properties of Vanadyl Porphyrins as Molecular Spin Qubits.

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Vanadyl (VO) porphyrins exhibit unique electronic and magnetic properties that make them promising candidates for molecular spin qubits. However, key magneto-structural parameters—including coherence times, spin transition accessibility, and spin-spin interactions—remain underexplored. This project aims to establish a foundational understanding of the magnetic properties that influence quantum coherence in VO porphyrins, focusing on VO petroporphyrin models. Initial efforts are focused on evaluating the coherence properties of substituted VO porphyrins and probing their potential as multi-level electronuclear qudits through nuclear spin state coupling. Electron paramagnetic resonance (EPR) spectroscopy is used to investigate the relationship between molecular structure and spin relaxation behavior. Data analysis routines are currently under development to enable effective comparison of spin relaxation as a function of porphyrin substitution. This project also aims to lay the groundwork for probing inter-porphyrin spin communication in VO porphyrin dimers. In addition to its scientific aims, this project provides undergraduate researchers with training in spectroscopy, computational tools, and quantitative data analysis. By integrating experimental approaches with theoretical insights, this work contributes to the broader understanding of transition metal-based molecular qubits and helps define a framework for future metalloporphyrin-based quantum architectures.

POSTER SESSION

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221 Q-band Double Quantum Coherence ESR for Sensitive Nitroxide-based Distance Measurements.

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Recent advances in pulsed dipolar spectroscopy have driven the sensitivity of the technique to physiologically relevant concentrations and extended the applicability to more complex biological systems. The most dramatic improvements in sensitivity have been achieved using orthogonal spin labeling strategies, however, a large majority of ESR applications involves dual nitroxide labels. In our recent breakthrough, we demonstrated Q-band nitroxide double quantum coherence (DQC) ESR for the first time, highlighting deep dipolar modulations of

100% and the ability to resolve multimodal distance distributions. In this work, we further establish DQC at Q-band as a practical technique for distance measurements in doubly nitroxide-labelled proteins. We show that 8 ns ? pulses provide efficient excitation of the double quantum transition at Q-band, though more commonly accessible pulse lengths also yield strong DQC signals. With optimized spectrometer tuning, we achieved signal-to-noise ratios exceeding 100 in just eleven minutes of acquisition for a dipolar evolution time of 1.5 μs for 50 ?M protein samples. We demonstrate the effects of deuteration on sensitivity of the DQC signal, which can further extend dipolar evolution times and the measurable distance range. The DQC results closely match recent theoretical predictions and reveal minimal background contributions from intermolecular interactions, even at concentrations up to 100 ?M. These findings highlight the advantages Q-band DQC for dual nitroxide-labelled proteins, including deep dipolar modulations, low background at micromolar concentrations, and improved sensitivity through deuteration. Collectively, our work positions Q-band nitroxide DQC as a powerful and accessible technique for pulsed ESR distance measurements.

POSTER SESSION

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222 Towards Quantum Diamond Microscope for Real-space, Wide-field Hyperpolarized NMR Imaging.

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Nuclear Magnetic Resonance at low magnetic fields is limited by poor signal-to-noise ratio due to weak thermal spin polarization, constraining its utility for microscale applications. While Dynamic Nuclear Polarization (DNP) can enhance signal strength by over an order of magnitude, it is commonly implemented with high-field, cryogenic, or inductive detection systems [1]. This project investigates the integration of DNP-enhanced spin polarization with a Radio Frequency Quantum Diamond Microscope (RF-QDM), an optical magnetometry platform based on Nitrogen-Vacancy (NV) centers in diamond. The RF-QDM enables wide-field (300 × 300 μm^2) narrowband magnetic imaging of both phase and amplitude by leveraging a lock-in camera for optical detection [2]. This approach achieves spectral resolution near 1 Hz, spatial resolution of 2 μm, and per-pixel magnetic sensitivity down to 1 nT/?Hz². A microfluidic sample delivery system is under development to interface hyperpolarized analytes with the NV diamond sensor surface, enabling label-free detection of NMR spectra and T? relaxation dynamics across the field of view. This platform allows for spatial mapping of chemical shift and J-coupling, supporting real-time, high-resolution NMR studies of micron-scale samples, opening new possibilities for metabolomics, reaction monitoring, and lab-on-chip diagnostics.

POSTER SESSION

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223 Photogenerated Spin-Correlated Radical Pairs in Silicon Quantum Dot– Organic Molecule Conjugates.

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The spin polarization exhibited by photogenerated spin-correlated radical pairs (SCRPs) make them attractive candidates for applications in spintronics and quantum sensing[1]. The spin states of these systems can be investigated and controlled using microwave pulses via electron paramagnetic resonance spectroscopy. Recent studies on metal-chalcogenide or metal-oxide based quantum dot–organic molecule conjugates have demonstrated the formation of photogenerated spin polarized states[2,3]. However, silicon quantum dots (Si QDs) present a more environmentally friendly and scalable alternative, offering tunable electronic properties while being compatible with existing semiconductor technologies[4]. In this study, we synthesized Si QD–NDI (naphthalene diimide) conjugates and demonstrated their ability to generate spin-polarized radical pairs through light-induced electron transfer. NDI was chosen for its low-lying acceptor states for efficient charge separation[3], while Si QDs have promising spin properties with size-tunable energy levels[4]. Time-resolved EPR (trEPR) spectra, obtained under 480 nm laser illumination at 20 K, confirm SCRP formation, indicating light-induced electron transfer rather than triplet energy transfer. The field positions, line shapes, and polarization patterns in trEPR data suggest that the charge-separated state originates from the excited state of Si QD, leading to electron transfer to NDI and the formation of a Si QD$^+$ and NDI$^-$ radical pair. These findings establish Si QD-NDI conjugates as a promising platform for spin-polarized charge transfer studies, offering an alternative to metal-based quantum dots.

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POSTER SESSION

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224 Detection of Multiple Components in Closely Spaced DEER Distance Distributions via Continuous Wavelet Transform.

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Identifying the presence of multiple components in DEER spectroscopy proves challenging with traditional P(r) methods when distances are closely spaced, requiring alternative approaches with pure component references. We demonstrate a frequency-domain method using Continuous Wavelet Transform (CWT) coupled with Structural Similarity Index Metric (SSIM) that requires pure component references to detect mixture compositions in systems with different component ratios. Using stilbestrol (2.2 nm) and estriol (2.0 nm) as references, we analyze mixtures across concentration ratios from 100:0 to 10:90 where P(r) analysis cannot identify individual components. CWT spectrograms reveal persistent frequency signatures for each component (stilbestrol at scale 20, estriol at scale 18) that remain detectable even when one component is present at only 10% concentration. As component ratios change, distance distributions evolve from unimodal to bimodal, yet localized SSIM comparison against pure references consistently confirms the presence of both components across all tested ratios. This reference-dependent approach enables component detection in closely spaced binary mixtures where conventional distance distribution methods cannot identify individual contributions.

POSTER SESSION

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225 Electrostatics of the Membrane Interface Revealed by EPR of Lipid-Based pH-Sensitive Probes.

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Electrostatic interactions are fundamental forces governing the behavior of charged molecules at the lipid membrane interface. These interactions, among other factors, influence ion distribution, membrane protein orientation, and ion channel activity. The electrostatic properties of lipid bilayers are dictated by fixed surface charges and quantitatively characterized by the surface electrostatic potential (?). One method for assessing surface electrostatics involves determining the electrostatic contribution to the pK_a shift of protonatable molecular probes positioned at the lipid bilayer interface. Previously, we successfully employed phospholipids head group-tagged with pH-sensitive nitroxide to map bilayer interfacial electrostatics by using EPR spectroscopy. As a further development of this methodology, we recently introduced an approach for determining the ionization constants of the EPR pH probes from the changes in their molecular tumbling upon protonation. Here we report on the application of this concept in a comparative study of the surface electrostatics of multilamellar (MLVs) and unilamellar vesicles (ULVs) composed of either 1-palmitoyl-2-oleoyl-sn-glycero-3-phospho-(1?-rac-glycerol) (POPG) or 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) lipids. Additionally, we demonstrate that this method can be expanded to experimentally discriminate surface electrostatics of the inner and outer leaflets of a lipid bilayer. The presented results further highlight the utility of the spin-labeled phospholipids in biophysical EPR spectroscopy and provide a deeper insight into the electrostatics of the lipid bilayer interface. This material is based upon work supported by the National Science Foundation under Grant No. 2305172.

POSTER SESSION

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226 OxyTrack: a Novel Needle Sensor for *in situ* Oximetry.

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A novel device for in situ oximetry, called OxyTrack, has been developed using OxyChip as the EPR oxygen-sensitive reporter. OxyTrack is a coax-tip resonator with an asymmetrical shunt between a grounded needle and an internal transmission line. The length of the transmission line between the needle tip and coupling capacitor determines the resonance frequency. The design has been tested with 300MHz pulse EPR as well as L-band and X-band CW EPR using the same resonator. Several OxyTrack designs have been constructed with needle outer diameter between 0.5–1 mm and needle length 3–17 cm and utilizing brass, nickel silver, or titanium outer needles. The following experiments were all conducted with a CW L-band instrument. The oxygen calibration was linear with standard error of inverse prediction (SEIP) 0.32 mmHg. OxyTrack showed excellent SNR at low power; SNR values of 86 and 144 were demonstrated at incident RF power of 45 and 126 nW, respectively. No significant change in signal intensity or measured linewidth was observed after insertion at depths up to 17 cm. In contrast, a standard surface resonator could measure signal up to only 5-mm deep using the same OxyChip reporter. It was also found that OxyTrack orientation with respect to the main magnetic field B_0 did not affect signal intensity or measured linewidth. Response of the OxyTrack to sudden change in oxygen concentration (between nitrogen and air oxygenation) took 60 seconds to reach equilibrium. The OxyTrack resonator was shown to be compatible with the medical imaging modalities CT and MRI. Finally, OxyTrack was used a mouse model of cancer (SCC7) to demonstrate differential response to 100% oxygen breathing in muscle and tumor. Overall, OxyTrack is an exciting new sensor for EPR oximetry.

POSTER SESSION

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227 Observation of Multi-mode Spin-Rabi Oscillation of Strongly EPR Driven Polaron Pairs In a Pi-Conjugated Polymer.

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Electron spin-Rabi oscillations electron paramagnetic-resonantly driven by a linearly polarized, strong radio-frequency domain magnetic field with amplitude B? that exceeds both, the static magnetic Zeeman field B? and the local random hyperfine field difference between polaron pair partners—have been predicted to give rise to long-lived charge carrier spin pair states.[1–3] These states are promising candidates for solid-state qubits due to their anticipated long coherence times and their potential for electrically readable single-spin detection.[4,5] To test the theoretical predictions in,[1] we performed strong-drive pulsed EPR experiments at room temperature using low-field (<0.5mT) pulsed electrically detected magnetic resonance (EDMR). Our measurements focused on spin-dependent polaron recombination currents in OLED devices based on deuterated poly[2-methoxy-5-(2'-ethylhexyloxy)-1,4-phenylenevinylene] (d-MEHPPV), which features reduced hyperfine interactions due to deuteration and thus, well-resolvable EPR peaks at Gauss-domain Zeeman fields. Experiments were conducted in regimes where B? = 0.67 mT, with B? = 0.36 mT (10 MHz) and B? = 0.72 mT (20 MHz). We observed that the integer number N of harmonics found in the Fourier spectrum of the Rabi nutation transient increases linearly with B?, following the relation 4B?/B?, predicted by theory,[1] with harmonics occurring at integer multiples of the drive frequency ?, decaying in a Bessel-function-like manner. Additionally, recombination suppression—a hallmark of strong-drive behavior—was observed over a broad range of B? and ?, in contrast to weak-drive regimes where such effects are confined near the on-resonance condition only.

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POSTER SESSION

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228 Rigid Cu(II) Spin Label Sensitive to DNA Conformational Flexibility in Protein-DNA Complexes.

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Measuring DNA conformation in protein-DNA complexes is essential for understanding how DNA structure and dynamics influence protein recognition and function. In this work, we introduce a new nucleotide-independent labeling strategy wherein Cu(II) is introduced directly within the DNA helix. The strategy utilizes two 8-aminoquinoline groups, one of each strand that rigidly anchors the Cu(II) ion within the DNA. The rigidity of the label allows us to accurately measure DNA conformations and dynamic fluctuations without convolution due to flexing of the label itself. To demonstrate the utility of the new label, we measure the changes in conformation of

DNA when it binds to type II restriction endonuclease EcoRV. The findings offer direct evidence in solution that the EcoRV endonuclease causes axial bending of DNA even without metal ions. Additionally, the narrowing of the distance distribution upon protein binding—and further with metal ion binding—suggests that the protein restricts the flexibility of the DNA helix. This approach presents a new and precise method to analyze DNA structure and dynamics in solution.

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POSTER SESSION

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229 Probing the Electrical Properties of Twisted Tetrathiafulvalene Thin-Films Using cwEPR.

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Tetrathiafulvalene (TTF) and its derivatives exhibit non-conventional optical and electrical properties.[1] As a result, the strong electron-donor TTF has been a cornerstone of the field of organic electronics. In recent work, optical activity has been imparted on polycrystalline TTF films by incorporation of a twisting agent, abietic acid. This modification results in a twisted TTF polymorph, exhibiting enhanced hole mobility.[2] Doping this polymorph with iodine further improves its conductivity through the oxidation of TTF. The temperature dependent conductivity of single crystal TTF iodine salts has been investigated previously, revealing conductivity in temperatures above 80 K result from a single spin species with large spin orbit coupling, as evidenced by its 180 G linewidth and 2.013 g-factor, to the iodine sublattice.[3] As part of this study we use a combination of conductivity measurements, variable temperature cwEPR and pulsed EPR at X-band to characterize the spin species that contribute to charge transport in iodine doped, twisted and non-twisted TTF thin films. The undoped non-twisted film exhibits an inhomogeneously broadened, 20 G wide, ESR signal at 296 K with a g-factor of ~ 2.011. As the twisted film is doped, two partially overlapping spin species with a Dysonian lineshape are observed, consistent with an increase in conductivity. The respective g-factors were determined to be ~2.017 and ~2.012. The increase in intensity of the EPR signal, due to doping, is incommensurate with the in-situ conductivity, suggesting the number of paramagnetic defects is not entirely responsible for the improved performance. The normalized intensity of the g ~ 2.017 species increases with temperature, suggesting thermal activation of the site. We investigate the sources of spin-lattice relaxation and coherence properties of the identified spin species as a function of temperature, and we compare these results to the observed conductivity.

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POSTER SESSION

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230 Enabling Enhanced Time-Resolved High-Field EPR of Protein Dynamics with a Quasioptical Sample Holder.

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Understanding protein function requires tools that can monitor site-specific conformational changes in real time. Most biophysical techniques rely on static snapshots or immobilized samples, limiting their ability to capture dynamic processes. Time-resolved electron paramagnetic resonance (EPR) spectroscopy overcomes this limitation by enabling real-time measurements of inter-residue distances in spin-labeled proteins1. Sherwin Lab has developed a rapid-scan, time-resolved EPR technique at 240 GHz—rsTiGGER—using Gadolinium(III) spin labels to probe protein dynamics2. A custom quasioptical sample holder featuring a roof-end mirror was central to this development, significantly improving signal-to-noise ratio (SNR) compared to previous designs3. This setup has successfully captured refolding dynamics of the J? helix in AsLOV22, but current limitations include poor temperature control and a time resolution ceiling of ~10 ms. Here, I present an updated quasioptical sample holder that addresses these constraints. The design incorporates a fine-threaded G10 differential screw (150 μm/turn) and a nanopositioning piezoelectric rotator for precision alignment of the roof mirror, enabling more consistent and reproducible optical coupling. The new coil holder is machined from Makor® machinable ceramic to reduce thermal conductivity, and a heat-sink resistor provides improved thermal control for temperature-sensitive samples. In parallel, to further boost SNR and approach sub-millisecond time resolution, we prototype a Fabry–Pérot-style sample capillary. This design uses indium tin oxide (ITO) coatings deposited onto rectangular borosilicate tubing to form partially reflective surfaces for standing-wave microwave enhancement. Together, these advancements in sample holder design push the limits of time-resolved high-field EPR, opening the door to probing fast, transient structural transitions in proteins with improved sensitivity and temporal resolution.

POSTER SESSION

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231 High Frequency NMR Spectroscopy With NV Centers in Diamond.

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Nuclear magnetic resonance spectroscopy is a powerful and widely used tool in the fields of chemistry, biology and pharmaceutical research. However, many applications in these fields demand very high spatial resolution are extremely sample limited to the degree where convetional inductive detectors struggle to deliver the necessary performance. The nitrogen-vacancy defect in diamond is a promising alternative as a platform for an NMR spectrometer capable of scaling to ? 1 nL sample volumes. Previous realizations of NV based NMR spectrometers have relied on dynamic-decoupling protocols synchronized with the Larmor precession of nuclear spins to detect the weak nuclear signals. The sensitivity of these mehtods scale poorly when increasing the bias magnetic fields to the level that is necessary to resolve the complex spectra that are often encountered in biological samples. In this work we propose an alternative sensing scheme called "Ramsey-M_z", which relies on detecting the longitudinal component of the nuclear magnetization and has a much improved sensitivity scaling with magnetic field.

POSTER SESSION

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232 EPR and Computational Study on the Radiation-induced Transformations in the Nuclear Fuel Cycle.

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Extraction separation plays a crucial role in the nuclear fuel cycle by utilizing specific organic ligands designed to selectively recover fuel components and radioactive fission products from waste solutions. Additionally, supplementary compounds are employed to regulate process conditions, including pH and preventing third-phase formation. Among the chemical classes commonly utilized are phosphoric acid esters (e.g., tributyl phosphate [TBP], dioctyl phosphate [DOP]), phosphine oxides (e.g., octyl(phenyl)-N,N-diisobutylcarbamoylmethylphosphine oxide [CMPO]), phosphonates (e.g., dibutyl((diethylamino)carbonyl)phosphonate [DBDECP]), diglycolamides (e.g., N,N,N?,N?-tetraoctyl diglycolamide [TODGA]), N,N-dialkyl amides (e.g., N,N-bis(2-ethylhexyl)butanamide [DEHBA], di-2-ethylhexylisobutyramide [DEHiBA]), carboxylic acids (e.g., oxalic acid [OA], lactic acid [LA], citric acid [CA]), and acetohydroxamic acid (AHA).

Considering these ligands are exposed to ionizing radiation, their radiolytic stability becomes a critical factor affecting extraction efficiency and solvent longevity. In this study, we present a comprehensive investigation of radiation-induced transformations of these ligands in both organic and aqueous phases using electron paramagnetic resonance (EPR) spectroscopy and quantum chemical calculations. The radiation-chemical yield of paramagnetic species in neat TBP exposed to X-rays was quantitatively assessed using the spin trapping method, although structural insights provided by this method remain limited. To clarify radical structures formed upon irradiation, we conducted EPR studies at 77 K on electron-beam irradiated ligands. In all cases, carbon-centered radicals were identified. Subsequent thermal annealing induced conformational relaxations without further chemical transformations.

In the aqueous phase, the radiolytic fate of ligands is influenced by reactions with water radiolysis products, particularly hydroxyl radicals. Using continuous-flow EPR spectroscopy, we investigated these reactions with selected organic acids, enabling the determination of radical structures, as well as their bimolecular decay kinetics.

POSTER SESSION

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233 Benchmarking Density Functional Theory for the Prediction of Fluoroalkyl Radical EPR Signatures.

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Per- and polyfluoroalkyl substances (PFAS) are among the most toxic, persistent, and bioaccumulative chemicals in widespread use today. Their exceptional chemical stability and surfactant properties have led to their incorporation into a wide range of consumer and industrial products, including food packaging, firefighting foams, and ski wax. However, these same properties have resulted in pervasive environmental contamination, prompting urgent and increasingly targeted efforts to remediate affected water and soil systems. Most current treatment strategies rely on oxidative or reductive processes to generate radical species capable of breaking the strong carbon–fluorine (C–F) bonds. Despite widespread assumptions that fluoroalkyl radical intermediates play a key role in these degradation pathways, they have yet to be directly observed under environmentally relevant conditions, leaving the underlying mechanisms of PFAS decomposition largely speculative. To address this knowledge gap and support future experimental investigations, we present the first systematic benchmarking study aimed at predicting the electron paramagnetic resonance (EPR) signatures of environmentally relevant fluoroalkyl radicals. This work provides calculations of ^{19}F hyperfine coupling constants and g-values for a series of small fluoroalkyl radicals, as well as for selected spin-trapped radical adducts. These results offer a critical foundation for designing EPR experiments capable of capturing fleeting radical intermediates and contribute to a more complete understanding of PFAS degradation mechanisms at the molecular level.

POSTER SESSION

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234 A Comprehensive Set of Distance Rulers for Pulse Dipolar ESR Spectroscopy.

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In order to further develop Pulse Dipolar ESR Spectroscopy (PDS), we synthesized and studied a number of rigid biradicals (“distance rulers”) with an interspin distance ranging from 1.5 to 3.9 nm. All synthesized biradicals show strong dipolar oscillation by PDS ESR, a typical Pake doublet pattern upon Fourier transform and a single interspin distance with sharp distance distribution P(r) after signal processing. In this presentation we show how these compounds were used to optimize experimental conditions for PDS spectroscopy, both DEER and DQC, as well as test systems in developing new data processing techniques and/or analyzing complex systems with multiple interspin distances. We also discuss special features of some of the radicals, for example trans/cis isomerization upon UV irradiation and their behavior in different solvents and polymer matrices. An important mission of ACERT is helping ESR users in the country and around the world. Based on our biradicals we manufactured a set of standards for PDS, “ACERT Rulers for ESR Distance measurements”, which we offer free of charge to the global ESR community. These standards are stable for years and can be used at room temperature.

POSTER SESSION

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235 Magnetic Resonance Spectroscopy of a Model Hydrogenase.

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Hydrogenases (H_2ases) are naturally occurring metalloenzymes that reversibly catalyze the hydrogen evolution reaction (HER) using only earth-abundant transition metals, namely iron and nickel.[1] [NiFe]-H_2ases, specifically, are less sensitive towards oxygen (O_2) than their [FeFe] counterparts, making them a better target for upscaling, though they are still susceptible to degradation upon prolonged exposure to O_2.[2] To avoid this problem, our research group has developed nickel-substituted rubredoxin (NiRd) as an electrocatalyst for HER under aerobic conditions.[3] We have shown that NiRd is a structural, functional, and mechanistic mimic of [NiFe]-H_2ases.[4] In this work, a suite of spectroscopic techniques was applied to primary and secondary sphere mutants of NiRd to elucidate mechanistic details and identify catalytically relevant cysteine residues. The ability to generate EPR-active Ni(I)Rd samples correlates with loss of HER activity in primary sphere mutants. Meanwhile, even though all secondary sphere mutants are catalytically active towards HER, the activities vary by over an order of magnitude. To understand how secondary sphere mutations affect HER activity, paramagnetic NMR spectroscopy was employed. Machine learning was used to extract important NMR parameters that relate to catalysis and reveal the importance of protein dynamics on the observed activity.

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POSTER SESSION

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236 High-field EPR Analysis of Co- and Fe-based Metal Complexes: Unraveling Electronic and Geometric Properties.

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Molecular spin qubits, known for their precise control and capability to sustain multiple quantum states, are poised to impact the field of quantum information science.[1,2] These qubits combine efficiency and versatility, allowing for large-scale production, precise tuning of spin environments, and arrangement in 2D or 3D lattices. Progress in their design and surface integration is crucial for overcoming challenges related to addressability, coherence, and scalability in future quantum systems. As a result, they represent a highly promising area for ongoing research and development in this cutting-edge field.

In this context, we performed high-field continuous-wave (CW) electron paramagnetic resonance (EPR) experiments at frequencies up to 413 GHz on Co- and Fe-based metal complexes to probe their electronic and structural properties. Specifically, we studied two Co(II) low-spin ($S = 1/2$) complexes, Co-SP and Co-TBP, both having the molecular formula [CoCl(DPPE)?]SnCl? but differing in geometry: Co-SP adopts a square pyramidal structure, whereas Co-TBP exhibits a trigonal bipyramidal arrangement. These distinct geometries substantially affect their electronic environments and resultant EPR signatures. The Co(II)-SP complex exhibits rhombic symmetry with g-values of 1.975, 2.245, and 2.32, while the Co(II)-TBP complex demonstrates axial symmetry with g-values of 2.035 and 2.232. Furthermore, high-power quasi-optical W-band spectrometer (HiPER) experiments revealed temperature-dependent relaxation behavior up to 60 K, with both complexes displaying similar characteristics when diluted. At 5 K, the spin-spin relaxation time (T_2) and spin-lattice relaxation time (T_1) for Co-TBP were approximately 5.8 μs and 0.62 ms, respectively, while Co-SP exhibited T_2 ? 3.5 μs and T_1 ? 0.98 ms. Additionally, we investigated a unique iron complex, [Fe???(L1)?][Na(DME)?], characterized by an unusual square planar geometry, providing valuable insights through detailed EPR analysis.[1]

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POSTER SESSION

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237 Time-resolved Electron Paramagnetic Resonance for Silicon Quantum Dots With Radical Organic Ligands.

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Silicon quantum dots (SiQDs) have arisen as a platform for quantum computing due to the ability for compactness over competing superconductor approaches used in industry, operational fidelity, the abundance of silicon, and performance at higher temperatures.[1]Currently, the central challenge of quantum information sciences is developing well-defined spin states that are available for coherent manipulation.[1] For this purpose, triplet states are postulated to be robust spin qubits with longer lifetimes and magnetic activity.[2]However, these states are optically dark but can be monitored through time-resolved electron paramagnetic resonance (trEPR) which can give information about electron transfer and spin dynamics in SiQD-conjugates.[3] The initial SiQD conjugates using 9-ethylanthracene and 9-vinylanthracene are utilized due to their efficient energy transfer.[4] The employment of radical ligands, such as phthalimide-N-oxyl (PINO) derivatives, 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO), and 9-azabicyclo[3.3.1]nonan-3-one-9-oxyl (KetoABNO), are desired to anchor to the SiQDs in order to test the spin-relaxation and coherence of these conjugates. These radicals were selected partly due to their nitroxide character which has been shown to have longer coherence times than most other types of radicals along with their rigidity which contributes to more efficient energy transfer.[5] Further, the doublet state of a radical can couple to the triplet which is generated from excitation of the SiQD to create a triplet-doublet state or the triplet can interact with two radicals separately and create a triplet-quartet state, both of which lead to longer coherence times and multi-level spin manifolds.[6] Motivated by these principles, in this study, we will explore the spin-relaxation times, coupling, and extent of delocalization for SiQD-organic conjugates, including a PINO derivative, TEMPO, and KetoABNO along with SiQD-9EA/9VA molecules. We will show results from trEPR experiments of these compounds in order to investigate how the different ligands affect the properties and longevity of the excited state.

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POSTER SESSION

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INDEX OF PRESENTERS

Name	Abstract No.
Aiello, Maxwell	135
Akhmetzyanov, Dmitry	200
Amassah, Georgina	201
Assafa, Tufa	123
Atwood, Sabastian	202
Avalos, Claudia	158
Aviles, Kristen.	131, 203
Bernd, Casey	204
Bindra, Jasleen	157, 205
Bittner, William	119, 206
Blank, Aharon	104
Bodenschatz, George	207
Boschmann, Sergius	115
Bowman, Michael	120
Budil, David	113
Burgess, Kaila	208
Carmielli, Raanan	109
Chauvire, Timothee	129, 209
Cheng, Emily	210
de Lima, Luan	211
Eaton, Gareth	117
Epel, Boris	100
Freed, Jack	133
Gamble Jarvi, Austin	212
Giovannone, Alex	139
Grimm, Brittany	130
Halpern, Howard	132
Hasanbasri, Zikri	107, 213
Hasany, Mariam	214
Hovey, Tanden	149
Hunter, Hannah	126, 215
Iqbal, Sehrish	216
Kay, Christopher	138
Kopp, Sebastian	136
Kotecha, Mrignayani	148, 217
Kroenke, Christopher	150
Krzyaniak, Matthew	154
Kuppusamy, Periannan	147
Le, Hoang	153, 218
Lerch, Michael	125
Lin, Wei-Hsu (Wish)	219
Lockart, Molly	220
Lowe, Eric	106
Mandato, Alysia	145, 221
Matheny, Julie	128
McDonnell, Camille	222
Mir Mohammadi, Seyedeh Shadi	223
Misra, Utkarsh	224
Nakamura, Toshikazu	118
Nguyen, Ngan	225
Niklas, Jens	111
O'Connell, Ryan	102,226
Odeke, Bonaventure	156,227
Ohta, Hitoshi	140
Pak, Chanhyun	137
Palit, Shramana	127,228
Poluektov, Oleg	155
Poudel, Prashanna	114
Qin, Peter	146
Ross, Matthew	116, 229
Schiemann, Olav	142
Schubert, Johanna	230
Sherwin, Mark	105
Silakov, Alexey	143
Sinha Roy, Aritro	144
Smirnov, Alex	122
Smirnova, Tatyana	124
Smits, Janis	231
Sosulin, Ilya	103, 232
Spackman, Isaac	233
Srivastava, Madhur	234
Srivastava, Nimesh	141
Straub, Joshua	152
Szalai, Veronika	121
Tait, Claudia	108
Teferi, Mandefro	110
Teptarakulkarn, Pathorn	235
Thangavel, Kavipriya	236
Tkach, Igor	151
Tseytlin, Mark	101
van Tol, Johan	134
Yount, Alexander	237
Yuen-Zhou, Joel	112