65th Annual

ROCKY MOUNTAIN CONFERENCE

ON MAGNETIC RESONANCE

Conference Program

and Abstracts

August 2-6, 2026

snowbird

Snowbird Resort and Conference Center
Snowbird, Utah

47th International EPR Symposium
Solid-state NMR Symposium

rockychem.com

65th ROCKY MOUNTAIN CONFERENCE ON MAGNETIC RESONANCE
August 2-6, 2026
Snowbird Resort & Conference Center, Snowbird, Utah

47th International EPR Symposium
Solid-state NMR Symposium

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www.rockychem.com ◆ info@rockychem.com

ORGANIZERS AND CHAIRPERSONS

CONFERENCE CHAIR:

Kurt W. Zilm
Yale University, Department of Chemistry PO Box 20817 • New Haven, CT 06520-8107
Ph: 203-432-3956 • Fax: 203-432-6144 • kurt.zilm@yale.edu

EPR SCIENTIFIC COMMITTEE

Mrignayani Kotecha (Chair)
O2M Technologies, LLC

Chandrasekhar Ramanathan (Vice Chair)
Dartmouth College

Victor Acosta
University of New Mexico

Chris Boehme
University of Utah

Sandra Eaton
University of Denver

Martyna Elas
Jagiellonian University

Songi Han
Chair Northwestern University

Petr Neugebauer
Central Euro. Inst. of Tech.

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University of Pittsburgh

Alexey Silakov
Penn State University

Stefan Stoll
University of Washington

Mark Tseytlin
West Virginia University

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Pierre et Marie Curie University

Björn Corzilius
Universität Rostock

Galia Debelouchina
University of California San Diego

Ulla Gro Nielsen
Novo Nordisk Foundation

Joanna Long
University of Florida

Aaron Rossini
Iowa State University

Ansgar Siemer
University of Southern California

CONFERENCE MANAGEMENT & TECHNOLOGY:

EVENT FLOW PROFESSIONALS | info@eventflowpros.com
WE KEEP EVENTS FLOWING

ROCKY MOUNTAIN CONFERENCE INFORMATION

REGISTRATION

Admission to all technical sessions and the exhibition is by name badge only.

Registration hours:

Sunday	Monday-Wednesday	Thursday
August 2	**August 3, 4, & 5**	**August 6**
10:00 AM–5:00 PM	8:00 AM–5:00 PM	8:00 AM–10:00 AM

EXHIBITION SCHEDULE

Monday	Tuesday	Wednesday
August 3	**August 4**	**August 5**
10:00 AM–7:00 PM	9:00 AM–5:00 PM	9:00 AM–4:00 PM

CONFERENCE RECEPTION

Monday evening from 5:30 PM to 7:00 PM, Ballroom 3 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 BANQUET & AWARDS CEREMONY

Wednesday from 7:00 PM to 9:00 PM in the **Conference Center Tent**. Enjoy an evening of comradeship, fine food and recognition of peers. Pre-registration required.

CONFERENCE LUNCH

A complimentary lunch is being provided August 3, 4, and 5 in **Golden Cliff (L1)/Eagles Nest (LL)/Superior Lobby (LL)** to all registered conference attendees from 12:00 PM to 1:30 PM.

ALTITUDE

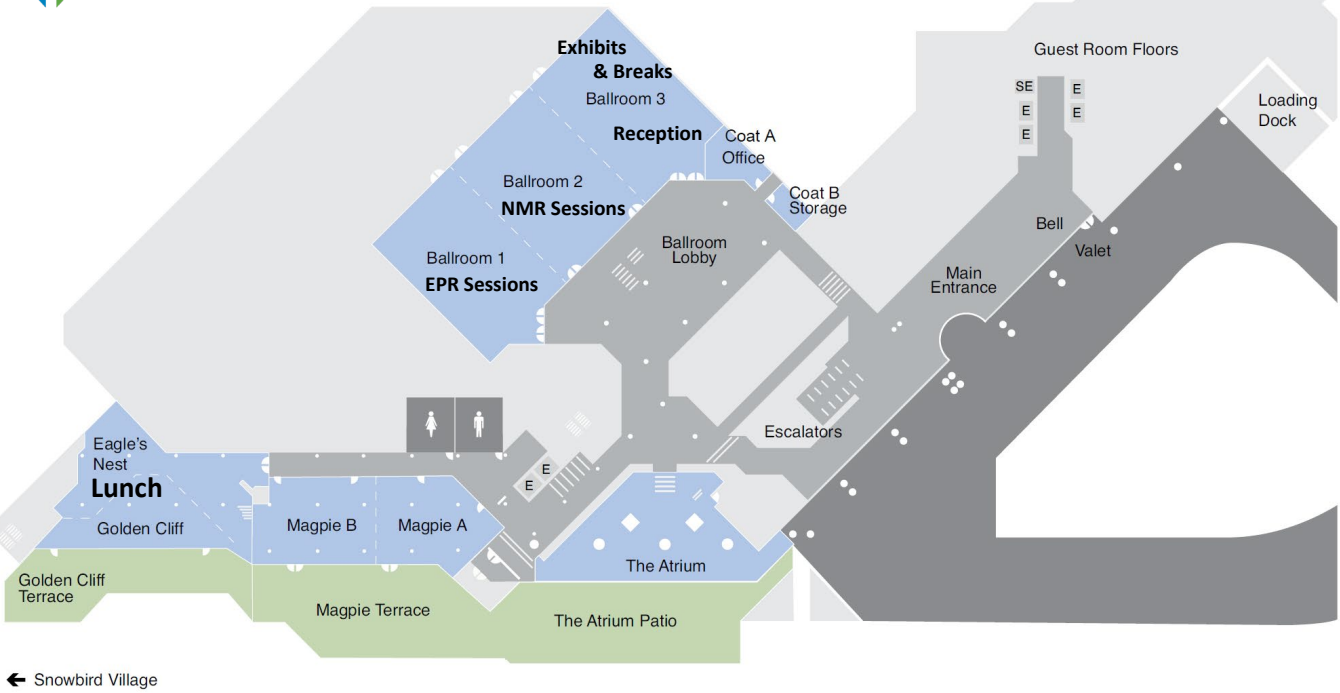
Snowbird is approximately 8,100 feet above sea level. The acclimatization process is inhibited by dehydration, over-exertion, alcohol and other depressant drugs.

Please take the following precautions regarding high altitude:

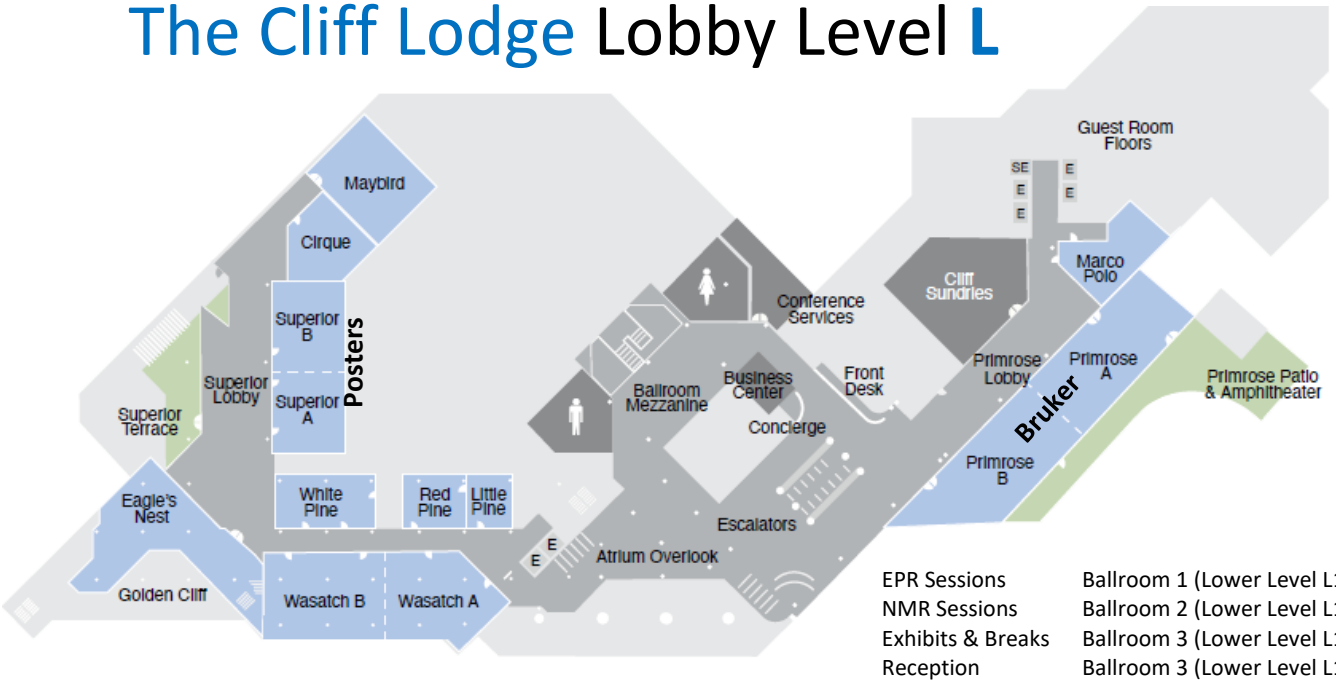
- Take it easy; don't over-exert yourself
- Light activity during the day is better than sleeping because respiration decreases during sleep, exacerbating the symptoms.
- Avoid tobacco, alcohol, and other depressant drugs including, barbiturates, tranquilizers, and sleeping pills.
- Eat a high carbohydrate diet
- Drink three to four times more water than usual

CONFERENCE SUPPORTERS

The Cliff Lodge Lower Level L1



The Cliff Lodge Lobby Level L



EPR Sessions	Ballroom 1 (Lower Level L1)
NMR Sessions	Ballroom 2 (Lower Level L1)
Exhibits & Breaks	Ballroom 3 (Lower Level L1)
Reception	Ballroom 3 (Lower Level L1)
Bruker	Primrose (Lobby Level L)
Lunch	Golden Cliff (L1) & Eagles Nest (Level LL)
Banquet	Conference Center Tent (Level 1)
Poster Session	Superior (Lobby Level L)

EXHIBITORS

CLIFF BALLROOM 3

Monday, August 3 10:00 AM–7:00 PM
Tuesday, August 4 9:00 AM–5:00 PM
Wednesday, August 5 9:00 AM–4:00 PM

ColdEdge Technologies

905 Harrison St, STE 146
Allentown, PA 18103
United States
Phone: +1 610-628-6363
sales@ColdEdgeTech.com
ColdEdgeTech.com

Booth 1

Resynant

8001 Terrace Ave, 203C
Middleton, WI 53562
United States
info@resynant.com
resynant.com

Booth 2

Doty Scientific, Inc.

700 Clemson Rd
Columbia, SC 29229
United States
Phone: +1 803-788-6497
sales@dotynmr.com
dotynmr.com

Booth 3

JEOL

11 Dearborn Rd
Peabody, MA 01960
United States
Phone: +1 978-535-5900
salesinfo@jeol.com
jeolusa.com

Booth 4

Bruker

15 Fortune Dr
Billerica, MA 01821
United States
Phone: +1 978-667-9580
info@bruker.com
bruker.com

Booths 5 & 6

PhoenixNMR LLC

510 E 5th St
Loveland, CO 80537
United States
Phone: +1 970-472-0613
info@phoenixnmr.com
phoenixnmr.com

Booth 7

PhoenixNMR LLC

No.1969, Kongquetai Rd,
High-tech Zone
Hefei, Anhui 230088 China
+86 130 8319 1369
info@ciqtek.com
ciqtekglobal.com

Booth 8

CIQTEK

3 Highwood Drive
Tewksbury, MA 01876
United States
Phone: 1-800-322-1174
cilsales@isotope.com
isotope.com

Booth 9

Cambridge Isotope Laboratories, Inc.

485 Wes Graham Way
Waterloo, ON N2L 0A7
Canada
Phone: +1 443-966-4211
info@highqtechnologies.com
highqtechnologies.com

Booth 10

High Q Technologies

1245 Ivy Street
Denver, CO, 80220
United States
Phone: +1 980-422-4723
shashwata@cryogenic-usa.com
cryogenic.co.uk

Booth 11

ACERT

1901 Pennsylvania Ave NW
Washington D.C. USA
United States
Phone: +1 202-770-2756
contact@acertcenter.org
acertcenter.org

Booth 12

Booth 1

Booth 10

CONFERENCE-AT-A-GLANCE

Sunday, August 2	Monday, August 3	Tuesday, August 4	Wednesday, August 5	Thursday, August 6
REGISTRATION				
Registration 10:00 AM - 5:00 PM	**Registration** 8:00 AM - 5:00 PM	**Registration** 8:00 AM - 5:00 PM	**Registration** 8:00 AM - 5:00 PM	**Registration** 8:00 AM - 10:00 PM
SCHEDULE				
	Exhibition (Ballroom 3) 10:00 AM – 7:00 PM	**Exhibition** (Ballroom 3) 9:00 AM – 5:00 PM	**Exhibition** (Ballroom 3) 9:00 AM – 4:00 PM	
Bruker SSNMR Workshop (Primrose) 7:30 AM – 12:15 PM	**Lunch** (Golden Cliff/Eagles Nest) 12:00 PM – 1:30 PM	**Lunch** (Golden Cliff/Eagles Nest) 12:00 PM – 1:30 PM	**Lunch** (Golden Cliff/Eagles Nest) 12:00 PM – 1:30 PM	
EPR Sunday Workshop (Ballroom 1) 2:00 PM - 5:00 PM	**EPR Lecturers** (Ballroom 1) 8:30 AM – 5:00 PM	**EPR Lecturers** (Ballroom 1) 8:30 AM – 5:00 PM	**EPR Lecturers** (Ballroom 1) 8:30 AM – 5:00 PM	**EPR Lecturers** (Ballroom 1) 8:30 AM – 12:00 PM
NMR Sunday Workshop (Ballroom 2) 1:30 PM - 4:00 PM	**NMR Lecturers** (Ballroom 2) 8:30 AM – 5:00 PM	**NMR Lecturers** (Ballroom 2) 8:30 AM – 5:00 PM	**NMR Lecturers** (Ballroom 2) 8:30 AM – 5:00 PM	**NMR Lecturers** (Ballroom 2) 8:30 AM – 12:00 PM
Bruker EPR User Meeting (Primrose) 5:30 PM – 9:30 PM	**Conference Reception** (Ballroom 3) 5:30 PM – 7:00 PM			
	Poster Session 1 (Superior) 7:00 PM – 9:00 PM	**Poster Session 2** (Superior) 7:00 PM – 9:00 PM	**Conference Banquet & Awards Ceremony** (Conference Center Tent) 7:00 PM – 9:00 PM	

CONFERENCE HIGHLIGHTS

SUNDAY, AUGUST 4, 2026

Bruker SSNMR Workshop:
7:30 AM - 12:15 PM (Primrose)
For information and registration access: REGISTER HERE

NMR Workshop:
Probe Building
(Rachel Martin)
1:30 PM – 4:00 PM (Ballroom 2)

EPR Workshop:
Low field experimental pulse EPR spectroscopy and imaging (O2M Technologies & FeMi Instruments)
2:00 PM – 5:00 PM (Ballroom 1)
For information and registration access:
https://oxygenimaging.com/events/rmc-epr-workshop-2026/

Bruker EPR User Meeting:
5:30 PM – 7:45 PM Meeting (Primrose)
7:45 PM – 9:30 PM Reception (Primrose)
For information and registration access: REGISTER HERE

MONDAY, AUGUST 5, 2026

Conference Reception
5:30 PM – 7:00 PM (Ballroom 3)
Check out all of the latest products and services as the reception is held right in the exhibition area.

TUESDAY, AUGUST 6, 2026

IES Award Lecture
8:30 AM (Ballroom 1)

WEDNESDAY, AUGUST 7, 2026

The Vaughan Lecture
1:00 PM – 4:30 PM (Ballroom 2)

Conference Banquet & Awards Ceremony:
7:00 PM - 9:00 PM (Conference Center Tent)
Pre-registration required.
- Banquet Speaker:
  Daniella Goldfarb - Weizmann Institute of Science
- EPR Awards
- SSNMR AWARDS

EPR SYMPOSIUM ORAL SESSIONS AGENDA

SUNDAY, AUGUST 2, 2026 EPR

EPR Workshop	**Low field experimental pulse EPR spectroscopy and imaging** **Ballroom 1**
	Jointly organized by O2M Technologies and FeMi Instruments, Chicago, IL ***Register here: https://oxygenimaging.com/events/rmc-epr-workshop-2026/*** ***Registration is only for planning purpose.***
2:00 – 3:00 PM	**Instrumentation with SpecMan4EPR: Spectroscopy and Imaging Experiments**. Boris Epel • Features of SpecMan4EPR (30 min) • Download and run dummy experiments, emulate spectroscopy (FID, 2 ENDOR lines, powder pattern), etc. • Demo of FeMiAWG • AI controlled SpecMan4EPR experiment demo • Q&A
3:00 – 3:15 PM	Break
3:15 – 3:40 PM	**JIVA-25 - pulse mode EPR imaging and applications.** Mrignayani Kotecha
3:40 – 4:10 PM	**Introduction to JIVA-MFI – Combined CW, MH, Rapid Scan, and Pulse EPR at 25 mT.** Boris Epel
4:10 – 5:00 PM	**Practical guide for image processing, visualization, data analysis.** O2M Team Members (Demonstration using real-world in vitro and in vivo data)
Bruker	**Bruker EPR User Meeting** **Primrose (Lobby Level L)**
	Register and information here: https://www.bruker.com/en/news-and-events/events/rmc.html
5:30 - 6:00 PM	Welcome & Networking
6:00 - 6:10 PM	**The EPR Team: Your Support Network.** Thorsten Maly, Bruker
6:10 - 6:30 PM	**ELEXSYS E580: A Trusted Platform in New Configuration.** Sylwia Kacprzak, Bruker
6:30 - 6:40 PM	**Return of the Gradients: X-band EPR Imaging.** Thorsten Maly, Bruker
6:40 - 6:55 PM	**DNP: Using Electrons for Sensitivity Gains in Solid-State NMR.** Shane Pawsey
6:55 - 7:05 PM	**One Year of Compact-Q DEER: Progress, Performance, and Outlook.** Dmitry Akhmetzyanov, Bruker
7:05 - 7:15 PM	**Advancing the E780 and Streamlined Sample Handling.** Sylwia Kacprzak, Bruker
7:15 - 7:30 PM	**Bruker EPR Resonators: Extending your Capabilities.** Dmitry Akhmetzyanov, Bruker
7:30 - 7:45 PM	**Trust the Signal, Question the Noise.** Thorsten Maly, Bruker
7:45 PM	Ending Remarks - Thorsten Maly, Bruker
7:45 - 9:30 PM	Reception

S1: Materials - Stefan Stoll, Chair		**Ballroom 1**
8:30 AM	101	**Optically induced spin polarization in open-shell molecular systems at variable magnetic fields.** Claudia Avalos, New York University
9:00 AM	102	**Spectroscopic and Theoretical Investigations of Co(II) and Fe(II) Compounds with a N4S2 Coordination.** Sebastian Stoian, University of Idaho
9:15 AM	103	**Applied EPR for degradation mechanisms of per-and polyfluoroalkyl substances (PFAS): A scoping review.** Isaac Spackman, Colorado School of Mines
9:30 AM	104	**Very High Frequency (263 GHz) Pulse EPR Spectroscopy of High Spin Transition Metal Centers.** Zikri Hasanbasi, University of California - Davis
9:45 AM	105	**Room-Temperature Spin-Dependent Charge Carrier Transitions in Racemic and Chiral Polyacetylene (CH)x Thin-Film Diodes.** Chiranjibi Dhakal, University of Utah
10:00 AM		*Break*
S2: Oximetry/RS/Imaging - Mrignayani Kotecha, Chair		**Ballroom 1**
10:30 AM	106	**Noninvasive EPR Detection of Melanin in Skin Melanomas: Why It Matters, How It Works, and What It Reveals.** Bernard Gallez, UCLouvain
11:00 AM	107	**High Spatial Resolution Quantitative Oxygen Imaging Using Image Domain Averaging**. Boris Epel, University of Chicago & O2M Technologies, LLC
11:15 AM	108	**Noninvasive Assessment of Oxidative Stress in Normal and Diabetic Mice Wounds Using 1.0 GHz Rapid Scan EPR.** Hanan Elajaili, University of Colorado Anschutz Medical Campus
11:30 AM	109	**Ex Vivo Liver Electron Paramagnetic Resonance Oxygen Imaging for Optimization of Organ Preservation Time.** Irene Canavesi, O2M Technologies, LLC
11:45 AM	110	**Impact of Heisenberg exchange on nitroxide T1 in low viscosity solutions.** Gareth Eaton, University of Denver
12:00 PM		*Lunch (included with registration)*
S3: Structural Biology - Tatyana Smirnova, Chair		**Ballroom 1**
1:30 PM	111	**Mechanism of CRISPR Target Discrimination Revealed by Site-Directed Spin Labeling.** Peter Qin, University of Southern California
2:00 PM	112	**Order-of-Magnitude Sensitivity Gains in DEER via Dual-Mode PBG Resonators.** Alex Smirnov, North Carolina State University
2:15 PM	113	**Navigating the Challenges of Excitation: Modeling Orientationally Selective Pulsed Dipolar EPR.** Nicholas Moriglioni, University of Pittsburgh
2:30 PM	114	**Quantum Spin Coherences in Photosynthetic Reaction Center Proteins.** Jens Niklas, Argonne National Laboratory
2:45 PM	115	**X-band CW EPR Reveals Confined Water and Ice Embryos Inside AOT Reverse Micelles.** John Franck, Advanced Center for ESR Research and Technology
3:00 PM		*Break*
S4: Chemistry 1 - Chandrasekhar Ramanathan, Chair		**Ballroom 1**
3:30 PM	116	**Photogenerated spin polarization in quantum dot – molecule conjugates.** Jacob H. Olshansky, Amherst College
4:00 PM	117	**Understanding ESR-STM signatures of single spins at surfaces.** Uwe Gerstmann, Paderborn University
4:20 PM	119	**Organic Radical Dendrimers as Metal-Free T_1 MRI Contrast Agents**. Vega Lloveras, University of Barcelona, Institute de Ciència de Materials de Barcelona (ICMAB–CSIC)
4:40 PM	120	**Decoherence of Nitroxide Spin Labels On Proteins**. Stefan Stoll, University of Washington
5:00 PM		END OF ORAL PROGRAM
5:30 - 7:00 PM		**Conference Reception** *(included with registration)*
Posters		
7:00 – 9:00 PM		Authors Present for Posters Labeled A

S5: Joint Session EPR/SSNMR - Sunil Saxena, Chair		**Ballroom 1 & 2**
8:25 AM		Citation and Award Presentation
8:30 AM	EPR 121	**IES Award Lecture** **Following Oxygen: Translational Advances in EPR Oximetry from Molecular Probes to Clinical Applications.** Periannan Kuppusamy, Geisel School of Medicine at Dartmouth College
9:00 AM	NMR 321	**Fast and accurate NMR crystallography with Machine Learning Interatomic Potentials.** Frederic Mentink-Vigier, National High Magnetic Field Laboratory
9:30 AM	EPR 122	**Insights into Second-Shell Waters of Gadolinium Contrast Agents using Electron-Nuclear Double Resonance (ENDOR): Implications for Relaxivity and Dynamic Nuclear Polarization.** Martyna Judd, Northwestern University
9:45 AM	NMR 322	**Determination of Atomically Precise Models of CdSe Quantum Dots Using DNP-Enhanced REDOR Solid-state NMR Spectroscopy**. Anuluxan Santhiran, Iowa State University
10:00 AM		*Break*
S6: Joint Session EPR/SSNMR - Periannan Kuppusamy, Chair		**Ballroom 1 & 2**
10:30 AM	EPR 123	**EPR: Room-temperature hyperpolarization and its applications in quantum sensing.** Kenichiro Tateishi, RIKEN
11:00 AM	NMR 323	**NMR: Exploiting High-Spin Gd(III) Central Transition for reduced-power Pulsed DNP (NOVEL).** Kong Ooi Tan, École Normale Supérieure
11:30 AM	EPR 124	**Registered EPROI And Ultrasound Imaging for Monitoring Tumor Oxygenation and Therapy Response.** Gabriela Dziurman, Jagiellonian University
11:45 AM	NMR 324	**Dynamic Nuclear Polarization with 1.3 mm Diameter Diamond Rotors.** Nicholas Wiesner, Massachusetts Institute of Technology
12:00 PM		*Lunch (included with registration)*
S7: Structural Biology - Peter Qin, Chair		**Ballroom 1**
1:30 PM	125	**Characterization of the Cu(II)-NTA spin label on proteins by x-ray crystallography and electron paramagnetic resonance.** Oliver Ernst, University of Toronto
2:00 PM	126	**Electrostatic Environment in Phospholipid Vesicles: Layer by Layer, Inside and Out.** Tatyana Smirnova, North Carolina State University
2:15 PM	127	**Applications of EPR to Biopharma: Structure, Dynamics, and Equilibria of a Monomer-Dimer System by Pulsed Dipolar Spectroscopy.** Austin Gamble Jarvi, High Q Technologies
2:30 PM	128	**Atomistic pictures of slow protein conformational changes using EPR and simulations.** Shramana Palit, University of Pittsburgh
2:45 PM	129	**Direct Detection of Multiple Distance Peaks from Pulsed Dipolar Signals.** Utkarsh Misra, Cornell University
3:00 PM		*Break*
S8: Instrumentation/Technology - Bernard Gallez, Chair		**Ballroom 1**
3:30 PM	130	**A Modular Low-Power 329 GHz Platform for Integrated EPR, NMR, and DNP.** Oleksii Laguta, Brno University of Technology
4:00 PM	131	**Recent advances in EPR cryoprobes.** Mantas Simenas, Vilnius University
4:15 PM	132	**Improving the modulation in 4-pulse DEER with swept observer pulses**. Eric Lowe, University of Maryland, Baltimore County
4:30 PM	133	**Versatile High-Sensitivity EPR Using Superconducting Spiral Microresonators.** Gediminas Usevičius, Vilnius University
4:45 PM	134	**Microresonators for Small Volume X-band EPR Measurements of Aqueous Protein Samples.** Anand Anilkumar, Medical College of Wisconsin
5:00 PM		END OF ORAL PROGRAM
Posters		
7:00 – 9:00 PM		Authors Present for Posters Labeled B

S9: Methodology/Spin Probes - Ilia Kaminker, Chair		**Ballroom 1**
8:30 AM	135	**Operando Monitoring of the Growth of Lithium Metal Dendrites Using EPR-on-a-Chip (EPRoC).** Klaus Lips, Helmholtz-Zentrum Berlin
9:00 AM	135	**Probing Local Interactions in Biological Redox Proteins with HYSCORE Spectroscopy: From Semiquinone Studies to Photosynthetic Proteins**. Patryk Kuleta, Indiana University
9:15 AM	137	**Dual EPR spin probe and label approach resolves origins of protein and coupled solvent dynamics and confinement-induced folding in fibrillar amyloid-β(1-42)**. Hana Alsheikh, Emory University
9:30 AM	138	**Frequency-Agile Pulse Slicing for High-Field, High-Power, Pulsed Electron Spin Resonance.** Alex Giovannone, University of California - Santa Barbara
9:45 AM	139	**First Experience with Large Volume Resonators for EPR Oxygen Imaging.** Daniel J SantaLucia**,** O2M Technologies, LLC
10:00 AM		*Break*
S10: Quantum Devices - Chris Boehme, Chair		**Ballroom 1**
10:30 AM	140	**Molecular Hyperfine Qubits Based on Heavy Elements.** Stephen Hill, Florida State University and NHMFL
11:00 AM	141	**Elucidating Electronic Structure and Relaxation Pathways of Transition Metal Qubits via High Power EPR Spectroscopy.** Kavipriya Thangavel, National high Magnetic Field Laboratory
11:15 AM	142	**Multi-Mode Spin-Rabi Oscillation of Strongly EPR Driven Electron Spins Pairs in the Landau Zener Regime.** Bonaventure Odeke, University of Utah
11:30 AM	143	**Confining Molecular Spin Qubits in Two-Dimensional Solid-State Architectures.** Anna Champ, Columbia University
11:45 AM	144	**Photoexcited transient EPR of tetrakis(4-carboxyphenyl)porphyrin (TCPP), with differing ions, as ligands in zirconium MOFs towards quantum sensors and DNP transfer.** Wern Ng**,** University of California Berkeley
12:00 PM		*Lunch (included with registration)*
S11: Materials 2 - Claudia Avalos, Chair		**Ballroom 1**
1:30 PM	145	**Magnetic resonance studies of poly-rotaxanes based on inorganic rings.** Eric McInnes, The University of Manchester
2:00 PM	146	**LLM-Assisted Modular Instrumentation: ODNP as a Case Study.** Atahan Garip, Advanced Center for ESR Research and Technology
2:15 PM	147	**EPR Characterization of Redox- and Topology-Dependent Spin Coupling in Diboron-Incorporated Indenofluorenes.** Yujie Zhao, Massachusetts Institute of Technology
2:30 PM	148	**Electrically detected ferromagnetic resonance evidence for orbital angular momentum transport in an organic semiconductor.** Prashanna Poudel, University of Utah
2:45 PM	149	**Sub-Terahertz Characterization of Anodic Aluminum Oxide Wafers for use in Liquid Sample High-Field EPR Resonators.** Johanna Schubert**,** University of California, Santa Barbara
3:00 PM		*Break*
S12: Chemistry - John Franck, Chair		**Ballroom 1**
3:30 PM	150	**ACERT Center Presentation**
4:00 PM	152	**(online) EPR with Imaging for batteries.** Bingwen Hu, East China Normal University
4:30 PM		
5:00 PM		END OF ORAL PROGRAM
7:00 – 9:00 PM		**Conference Banquet & Awards Ceremony** (pre-registration required)
Enjoy an evening of comradeship, fine food, and recognition of peers. – ***Speaker: Daniella Goldfarb***		

S13: Quantum Devices 1/Methodology - Madhur Shrivastava, Chair		**Ballroom 1**
8:30 AM	153	**From diamond defects to protein-based qubit sensors.** Peter Maurer, The University of Chicago
9:00 AM	154	**Rotor-synchronized Magic Angle Spinning EPR Experiments at 7 and 14 Tesla.** Ilia Kaminker, Tel Aviv University
9:15 AM	155	**High field microfluidic NMR spectroscopy by longitudinal magnetization detection with pulsed NV magnetometry.** Janis Smits, University of New Mexico
9:30 AM	156	**Next-Generation EPR: Combining High-Performance Q Band Instrumentation with Artificial Intelligence Enhanced Spectral Processing.** Zhiyu Sun, CIQTEK
9:45 AM	157	**Fourier Transform EPR Spectroscopy Revisited.** Dmitry Akhmetzyanov**,** Bruker BioSpin Corp.
10:00 AM		*Break*
S14: Joint Session EPR/SSNMR – Boris Epel, Chair		**Ballroom 1**
10:30 AM	EPR 158	**Expanding Applications of EPR Oximetry with the Ox071 Spin Probe: From Tumor Oxygen Imaging to Detection of Kidney Injury.** Shun Kishimoto, NCI
11:00 AM	NMR 354	**High-Field MAS DNP toward In-Situ Amyloid Structural Biology.** Yoh Matsuki, The University of Osaka
11:40 AM	EPR 159	**Robust AC Vector Sensing with Pentacene and Enhancing Spin Coherence byNuclear Spin Hyperpolarization.** Yifan Quan, University of Pennsylvania
11:45 AM	NMR 355	**Unraveling Interactions in Heterogeneous Catalysts using Fast MAS Solid-State NMR and EPR Spectroscopy.** Amrit Venkatesh, University of Virginia
12:00 PM		**CONFERENCE CONCLUDES**

EPR POSTER SESSIONS

MONDAY, AUGUST 3 • 7:00 PM – 9:00 PM (*Authors Present for Posters Labeled A)*
TUESDAY, AUGUST 4 • 7:00 PM – 9:00 PM (*Authors Present for Posters Labeled B)*

ERP POSTER SESSIONS		
A	200	**Enhancing the Stability of BDPA Radicals through Chemical Design and Synthesis**. Abigail Von Niederhausern, Utah State University
B	201	**Physics-Constrained AI Framework for Robust and Distortion-Tolerant EPR Oxygen Mapping**. Irene Canavesi, Technion - IIT
A	202	**Electron Paramagnetic Resonance Spectroscopy for Evaluation of Free-Radical Scavenging Properties: a Comparative Study of Ascorbic Acid and Ketone Bodies**. Amarachi Emole, Steppingstone Magnetic Resonance Training (SMART) Center
B	203	**Microwave phase noise mitigation using double quantum coherent control of NV-centers in diamond**. Amilcar Jerónimo Pérez, University of New Mexico
A	204	**Confining Molecular Spin Qubits in Two-Dimensional Solid-State Architectures**. Anna Champ, Columbia University
B	205	**Applications of EPR to Biopharma: Structure, Dynamics, and Equilibria of a Monomer-Dimer System by Pulsed Dipolar Spectroscopy**. Austin Gamble Jarvi, High Q Technologies
A	206	**High Spatial Resolution Quantitative Oxygen Imaging Using Image Domain Averaging**. Boris Epel, O2M Technologies, LLC
B	207	**Measurement of TEMPO Reduction to Determine Storage Effects on Antioxidant Levels in Fruits and Vegetables III**. Emily Cheng, University of Michigan
A	208	**Improving the modulation in 4-pulse DEER with swept observer pulses**. Eric Lowe, University of Maryland, Baltimore County
B	209	**Dual EPR spin probe and label approach resolves origins of protein and coupled solvent dynamics and confinement-induced folding in fibrillar amyloid-β(1-42)**. Hana Alsheikh, Emory University
A	210	**Applied EPR for degradation mechanisms of per-and polyfluoroalkyl substances (PFAS): A scoping review**. Isaac Spackman, Colorado School of Mines
B	211	**Ex Vivo Liver Electron Paramagnetic Resonance Oxygen Imaging for Optimization of Organ Preservation Time**. Irene Canavesi, O2M Technologies, LLC
A	212	**High field microfluidic NMR spectroscopy by longitudinal magnetization detection with pulsed NV magnetometry**. Janis Smits, University of New Mexico
B	213	**Structural Characterization of the Cu(II)-NTA Spin Label on α-Helices by Electron Paramagnetic Resonance and X-ray Crystallography**. Joerg Reichenwallner, University of Toronto
A	214	**Exploring Matter Through Electron Spin Resonance: Tools and Opportunities at the NHMFL**. Johan van Tol, Florida State University
B	215	
A	216	**Elucidating Electronic Structure and Relaxation Pathways of Transition Metal Qubits via High Power EPR Spectroscopy**. Kavipriya Thangavel, National high Magnetic Field Laboratory
B	217	**L-band (1.0 GHz) Rapid-Scan EPR Spectroscopy and Imaging with a Surface Coil Resonator**. Liberty Debrah, University of Denver
A	218	**Probing Intermolecular Exchange Weak Interactions from Single Crystal HFEPR Measurements**. Luan Lima, Brno University of Technology (BUT)
B	219	**Insights into Second-Shell Waters of Gadolinium Contrast Agents using Electron-Nuclear Double Resonance (ENDOR): Implications for Relaxivity and Dynamic Nuclear Polarization**. Martyna Judd, Northwestern University
A	220	**Rabi Beat Spectroscopy of Spins Undergoing Fast Exchange**. Michael Bowman, The University of Alabama
B	221	**Polarization-Controlled Floquet Transitions in Strongly Driven Electron Spin Pairs**. Nathan Chanhyun Pak, University of Utah
A	222	**Navigating the Challenges of Excitation: Modeling Orientationally Selective Pulsed Dipolar EPR**. Nicholas Moriglioni, University of Pittsburgh
B	223	**Enhancing the Stability of BDPA Radicals through Chemical Design and Synthesis**. Olivia Woodward, Utah State University

A	224	
B	225	**The SMART Center: EPR Spectroscopy as a Teaching and Research Platform for the Broader Magnetic Resonance Community**. Reef (Philip D., II) Morse, Steppingstone Magnetic Resonance Training Center
A	226	**Small Changes in Stereochemistry, Large Effects on Membrane Organization: An EPR Study of Glucosylceramides**. Shayak Biswas, University of Florida
B	227	**Atomistic pictures of slow protein conformational changes using EPR and simulations**. Shramana Palit, University of Pittsburgh
A	228	**Decoherence of Nitroxide Spin Labels On Proteins**. Stefan Stoll, University of Washington
B	229	**Electrostatic Environment in Phospholipid Vesicles: Layer by Layer, Inside and Out**. Tatyana Smirnova, North Carolina State University
A	230	**Direct Detection of Multiple Distance Peaks from Pulsed Dipolar Signals**. Utkarsh Misra, Cornell University
B	231	**Organic Radical Dendrimers as Metal-Free T_1 MRI Contrast Agents**. José Vidal-Gancedo, Institut de Ciència de Materials de Barcelona (ICMAB–CSIC)
A	232	**Silicon L-Center Characterization via Orientation-Selective High-Field EPR**. Wei-Hsu Lin, UC Santa Barbara
B	233	**Photoexcited transient EPR of tetrakis(4-carboxyphenyl)porphyrin (TCPP), with differing ions, as ligands in zirconium MOFs towards quantum sensors and DNP transfer**. Wern Ng, University of California Berkeley
A	234	**Robust AC Vector Sensing with Pentacene and Enhancing Spin Coherence byNuclear Spin Hyperpolarization**. Yifan Quan, University of Pennsylvania
B	235	**EPR Characterization of Redox- and Topology-Dependent Spin Coupling in Diboron-Incorporated Indenofluorenes**. Yujie Zhao, Massachusetts Institute of Technology
A	236	**Next-Generation EPR: Combining High-Performance Q Band Instrumentation with Artificial Intelligence Enhanced Spectral Processing**. Zhiyu Sun, CIQTEK
B	237	**Very High Frequency (263 GHz) Pulse EPR Spectroscopy of High Spin Transition Metal Centers**. Zikri Hasanbasri, University of California – Davis
A	238	**ACERT: A Service Resource for ESR Researchers**. Madhur Srivastava, Cornell University

SSNMR SYMPOSIUM ORAL SESSIONS AGENDA

SUNDAY, AUGUST 2, 2026 SSNMR

Bruker	**Bruker SSNMR Workshop** **Primrose – Lobby Level L**
	Register and information here: https://www.bruker.com/en/news-and-events/events/rmc.html
7:30 -8:15 AM	Breakfast
8:15 - 8:20 AM	Welcome & Introductions. Shane Pawsey, Bruker
8:20 - 8:35 AM	Solids Update. Sebastian Wegner, Bruker
8:35 - 9:00 AM	**Tracking Electrolyte Decomposition and SEI Formation in Lithium-ion Batteries**. Emma McGee, McMaster University
9:00 - 9:25 AM	**Triple-Resonance (HFX) Enables Separation of 19F-Mediated Cross-Relaxation Pathways under DNP.** Edvards Bensons, University of Rostock
9:25 - 10:00 AM	**^{31}P Solid-State NMR of γ-Irradiated Rare-Earth Minerals**. Professor Claudia E. Avalos, New York University
10:00 - 10:30 AM	Break
10:30 - 10:50 AM	**Same Rotor, New Insight: Benchtop EPR for Quantitative Radical Concentration in DNP Samples.** Thorsten Maly, Bruker
10:50 - 11:15 AM	**Transceiver Coil Fabrication and Testing with Probe in a Box Benchtop Device**. Annie Victoria McAllister, University of California Irvine
11:15 - 11:40 AM	**Solid-State NMR Strategies to Characterize the Interactions Between Fluorescent Sensors and Mineral Surfaces**. Sophie Young, University of California San Diego
11:40 - 12:15 PM	**Resolution or Sensitivity? Contributions of (ultra) High Field NMR to Materials Science.** Pierre Florian, CEMHTI-CNRS, Orléans, France
NMR Workshop	**Ballroom 2**
1:30 – 4:00 PM	Probe Building – Rachel Martin

S1: Materials – Pierre Florian, Chair		**Ballroom 2**
8:30 AM	301	**MAS meets order – from oriented micro-crystals to secular dipolar order.** Kazuyuki Takeda, Kyoto University
9:00 AM	302	**Design of a Triple-Resonance (1H/13C/17O), Cryogenic, DNP-MAS Transmission Line Probe for an 800MHz Spectrometer.** Samuel Strymish, Massachusetts Institute of Technology
9:15 AM	303	**Advances in Sensitivity and Photoillumination Technology for Magic-AngleSpinning Probes.** Lauren Price, Resynant
9:30 AM	304	**Rethinking MAS NMR with Additive Manufacturing: Optimized 3D-Printed RF Coils and Single-Sided MAS of Planar Samples.** Thomas Osborn Popp, Oregon State University
9:45 AM	305	**Setting the Magic-Angle with a Probe-Integrated Independent NMR-Based Sensor.** Marcus Tuttle, PhoenixNMR LLC
10:00 AM		*Break*
S2: Biosolids – Rachel Martin, Chair		**Ballroom 2**
10:30 AM	306	**Explorations of membrane-active peptide partitioning, lipid phases, and pH in pulmonary surfactant**. Joanna Long, University of Florida
11:00 AM	307	**A Model for Solid-State NMR Studies of FG-Repeat Peptides under Nanopore Confinement.** Wancheng Zhao, National Institutes of Health
11:15 AM	308	**An eye lens protein forms a transparent gel via nonspecific transient interactions.** Jaewon Suk, University of California, Irvine
11:30 AM	309	**Lipid Regulation of Membrane Proteins as Observed by Solid State NMR.** Benjamin Wylie, Indiana University
11:45 AM	310	**α-Synuclein Membrane Binding with DNP NMR.** Sahil Ahlawat, UT Southwestern Medical Center
12:00 PM		*Lunch (included with registration)*
S3: Methods - Björn Corzilius, Chair		**Ballroom 2**
1:30 PM	311	**Magnetic Resonance Studies of Paramagnetic and Metallic Battery Materials.** Clare Grey, University of Cambridge
2:00 PM	312	**Mechanochemical Synthesis and Multinuclear Solid-State NMR Spectroscopy of Metal Coordination Compounds.** Jazmine Sanchez, Florida State University
2:15 PM	313	**Surface-Only NMR of Calcium Silicate Hydrate: Advancing Surface-Selective Methods to the Atomic-Level Surface Structure Of Cements.** Ray Cowen, EPFL
2:30 PM	314	**Measuring, Calculating, and Overcoming Large Anisotropies in Energy Materials.** Michael A. Hope, University of Warwick
2:45 PM	315	**Deciphering the Topology of Less Ordered Materials Using an NMR AssistedApproach.** Brijith Thomas, New York University Abudhabi
3:00 PM		*Break*
S4: Methods – Aaron Rossini, Chair		**Ballroom 2**
3:30 PM	316	**Combining CSA and Dipolar recoupling reveals a dynamic window in filamentous phage capsids.** Amir Goldbourt, Tel Aviv University
4:00 PM	317	**Influence of Paramagnetic Relaxation Additives on DNP-enhanced MAS NMR.** Ronja Roessler, University of Rostock, Germany
4:15 PM	318	**Nanosecond Electron Spin Dynamics in Diamond Probed by Pulsed DNP at 7 T.** Alexander Nevzorov, North Carolina State University
4:30 PM	319	**Solid-State NMR and DNP Investigation of PFAS Binding in Zr-Based MOFs.** Yifan Quan, University of Pennsylvania
4:45 PM	320	**A Proposed NMR Correction to the Crystal Structure of Cefdinir Anhydrate.** James Harper, University of Utah
5:00 PM		END OF ORAL PROGRAM
5:30 - 7:00 PM		**Conference Reception** *(included with registration)*
Posters		
7:00 – 9:00 PM		Authors Present for Posters Labeled A

S5: Joint Session EPR/SSNMR - Sunil Saxena, Chair		**Ballroom 1 & 2**
8:25 AM		Citation and Award Presentation
8:30 AM	EPR 121	**IES Award Lecture** **Following Oxygen: Translational Advances in EPR Oximetry from Molecular Probes to Clinical Applications.** Periannan Kuppusamy, Geisel School of Medicine at Dartmouth College
9:00 AM	NMR 321	**Fast and accurate NMR crystallography with Machine Learning Interatomic Potentials.** Frederic Mentink-Vigier, National High Magnetic Field Laboratory
9:30 AM	EPR 122	**Insights into Second-Shell Waters of Gadolinium Contrast Agents using Electron-Nuclear Double Resonance (ENDOR): Implications for Relaxivity and Dynamic Nuclear Polarization.** Martyna Judd, Northwestern University
9:45 AM	NMR 322	**Determination of Atomically Precise Models of CdSe Quantum Dots Using DNP-Enhanced REDOR Solid-state NMR Spectroscopy**. Anuluxan Santhiran, Iowa State University
10:00 AM		*Break*
S6: Joint Session EPR/SSNMR - Periannan Kuppusamy, Chair		**Ballroom 1 & 2**
10:30 AM	EPR 123	**EPR: Room-temperature hyperpolarization and its applications in quantum sensing.** Kenichiro Tateishi, RIKEN
11:00 AM	NMR 323	**NMR: Exploiting High-Spin Gd(III) Central Transition for reduced-power Pulsed DNP (NOVEL).** Kong Ooi Tan, École Normale Supérieure
11:30 AM	EPR 124	**Registered EPROI And Ultrasound Imaging for Monitoring Tumor Oxygenation and Therapy Response.** Gabriela Dziurman, Jagiellonian University
11:45 AM	NMR 324	**Dynamic Nuclear Polarization with 1.3 mm Diameter Diamond Rotors.** Nicholas Wiesner, Massachusetts Institute of Technology
12:00 PM		*Lunch (included with registration)*
S7: Biosolids/Methods – Joanna Long, Chair		**Ballroom 2**
1:30 PM	325	**Solid-State NMR and DNP Reveals Dynamic Lignin-Carbohydrate Architectures Across Plant Development and Carbon Cycling.** Tuo Wang, Michigan State University
2:00 PM	326	**Decoding Early Mineralization and Surface Layer Formation of Bone Mimetic Apatite Using Complementary Solution and Solid-State NMR.** Gil Goobes, BAR ILAN UNIVERSITY
2:15 PM	327	**NMR-Assisted Crystallography of Aspartate Aminotransferase: Protonation States and Catalytic Mechanism**. Paula Magat, University of California, Riverside
2:30 PM	328	**Cryogen-free magnets for solid-state MAS NMR at multiple magnetic fields.** Denis Langlais, Cryogenic US LLC
2:45 PM	329	**Probing the limits to refocusing nuclear spin dynamics.** Chandrasekhar Ramanathan, Dartmouth College
3:00 PM		*Break*
S8: Materials – Pierre Florian, Chair		**Ballroom 2**
3:30 PM	330	**Linking Structure, Dynamics, and Reactivity in Energy Storage Materials through Operando Solid-State NMR and Relaxometry.** Gillian Goward, McMaster University
4:00 PM	331	**Solid-state NMR spectroscopy of the platinum group elements and their replacements: experimental and computational advances.** Sean Holmes, Florida State University
4:15 PM	332	**A 1H NMR Investigation of a Birnessite-like MnOx Electrode Material.** Mark Bovee, U.S. Naval Research Laboratory
4:30 PM	333	**Structural Analysis of 13C and 15N Isotopically Labeled Chitin in its Natural Biological State via Solid-State NMR of Manduca sexta Pupal Cuticle**. William Nese, West Virginia University
4:45 PM	334	**Towards Microscale NMR at 14T using Quantum Diamond Sensors**. Chung Tung Cheung, University of Chicago
5:00 PM		END OF ORAL PROGRAM
Posters		
7:00 – 9:00 PM		Authors Present for Posters Labeled B

S9: Biosolids/Methods – Ansgar Siemer, Chair		**Ballroom 2**
8:30 AM	335	**Molecular-scale mapping of the Pseudomonas aeruginosa biofilm matrix.** Courtney Reichhardt, Washington University in St. Louis
9:00 AM	336	**Accelerating Protein NMR Crystallography with Machine-Learning Interatomic Potentials: Protonation States in the Active Site of Toho-1.** Len Mueller, University of California - Riverside
9:15 AM	337	**Magic-Angle Spinning Solid State NMR in a 5 mm Solution Probe via MAS-SPINDLE.** Ryan Galperin, Oregon State University
9:30 AM	338	**Mechanochemical Routes to Conventional and Integrative Pharmaceutical Solid Forms: Insights from PXRD and Multinuclear Solid-State NMR Spectroscopy.** Peyton Osborn, Florida State University & National High Magnetic Field Laboratory
9:45 AM	339	**Getting the most information out of quantum noise spectroscopy.** Andres Montoya Castillo, University of Colorado Boulder
10:00 AM		*Break*
S10: Materials – Aaron Rossini, Chair		**Ballroom 2**
10:30 AM	340	**NMR & MRI: More from Graph Theory, Path-Sum and Divided Difference Functions.** Christian Bonhomme, Sorbonne University
11:00 AM	341	**"Magic-angle hopping" Na-ion dynamics in a sodium antiperovskite: a distinct motional averaging mechanism of the quadrupolar interaction.** David Halat, Colorado School of Mines
11:15 AM	342	**Structure Determination of 2D Germanane, Methyl Germanane and Methyl Germanane-Stannane Nanosheets by Nuclear Magnetic Resonance Spectroscopy.** Lukman Yunusa, Iowa State University
11:30 AM	343	**Probing surface terminations and lithium intercalation in Ti3C2Tx MXene using ex situ NMR.** Ryan Bragg, University of Warwick
11:45 AM	344	**NMR Crystallography of Emerging Classes of Lithium and Sodium Transition-metal Oxide and Phosphate Materials.** Kent Griffith, University of California San Diego
12:00 PM		*Lunch (included with registration)*
Vaughan Lecture – Rachel Martin, Chair		**Ballroom 2**
1:30 PM	345	**Solid-State NMR Strategies for Probing Rare Earth Structure and Dynamics.** Brennan Walder, Ames National Laboratory
2:00 PM	346	**Multi-Nuclear Solid State NMR Studies of Structure-Property Relationships in Glass, with Applications Ranging from Nuclear Waste Storage to High-Performance Optics.** Ulrike Werner-Zwanziger, Dalhousie University
3:30 PM	347	**Structural Defects in Glass: are traditional models being called into question?** Pierre Florian, CEMHTI-CNRS
3:00 PM		*Break*
3:30 PM	348	**Inverse Methods for Nuclear Magnetic Resonance of Non-Crystalline Materials**. Philip Grandinetti, The Ohio State University
4:30 PM		END OF ORAL PROGRAM
7:00 – 9:00 PM		**Conference Banquet & Awards Ceremony** (pre-registration required)
Enjoy an evening of comradeship, fine food, and recognition of peers. – ***Speaker: Daniella Goldfarb***		

S11: Methods - Björn Corzilius		**Ballroom 2**
8:30 AM	349	**Chemical Shift Based Amino Acid-Type Spectral Editing for Backbone Atoms and Residue Centric Distance Restraint Mapping in Fast Magic Angle Spinning U-[13C,15N] Proteins.** Vipin Agarwal, TATA Institute of Fundamental Research
9:00 AM	350	**Repulsion-Driven Superionic Conductivity in La2Mo2O9 monitored by DFT-assisted NMR spectroscopy.** Adriana Bocchini, Paderborn University
9:15 AM	351	**Probing the local environment of quadrupolar isotopes in materials using ultra-high-field NMR and advanced pulse sequences.** Olivier Lafon, Univ. Lille
9:30 AM	352	**Interpreting chemical shielding tensors: a well-posed approach through real-space analysis.** Josef Zwanziger, Dalhousie University
9:45 AM	353	**1H led NMR Structure Determination in Molecular Solids.** Jacob Holmes, EPFL
10:00 AM		*Break*
S12: Joint Session EPR/SSNMR – Boris Epel, Chair		**Ballroom 1**
10:30 AM	EPR 158	**Expanding Applications of EPR Oximetry with the Ox071 Spin Probe: From Tumor Oxygen Imaging to Detection of Kidney Injury.** Shun Kishimoto, NCI
11:00 AM	NMR 354	**High-Field MAS DNP toward In-Situ Amyloid Structural Biology.** Yoh Matsuki, The University of Osaka
11:40 AM	EPR 159	**Robust AC Vector Sensing with Pentacene and Enhancing Spin Coherence byNuclear Spin Hyperpolarization.** Yifan Quan, University of Pennsylvania
11:45 AM	NMR 355	**Unraveling Interactions in Heterogeneous Catalysts using Fast MAS Solid-State NMR and EPR Spectroscopy.** Amrit Venkatesh, University of Virginia
12:00 PM		**CONFERENCE CONCLUDES**

SSNMR POSTER SESSIONS

MONDAY, AUGUST 3 • 7:00 PM – 9:00 PM (*Authors Present for Posters Labeled A)*
TUESDAY, AUGUST 4 • 7:00 PM – 9:00 PM (*Authors Present for Posters Labeled B)*

SSNMR POSTER SESSIONS		
A	400	**HTRA1 Forms Multimeric Assemblies with TDP-43: A Solid-State NMR Study**. Arshad Abdulvahid, University of Southern California
B	401	**23Na NMR Studies of Amorphous Chlorides for Solid-State Na-ion Batteries.** Kevin Anderton, University of California, San Diego
A	402	**A 1H NMR Investigation of a Birnessite-like MnOx Electrode Material**. Mark Bovee, U.S. Naval Research Laboratory
B	403	**Rethinking isotopic substitution for NMR studies: Impacts of deuteration on sodium dynamics in sodium amide borohydride**. Tyler Case, Colorado School of Mines
A	404	**Probing the Structures and Dynamics of Cobaltocenium Salts via Ultra-Wideline 59Co Solid-State NMR.** Dominic Chantra, Florida State University
B	405	**Surface-Only NMR of Calcium Silicate Hydrate: Advancing Surface-Selective Methods to the Atomic-Level Surface Structure Of Cements**. Ray Cowen, EPFL
A	406	**Utilizing 3D-Printing and Electroplating to Develop Solid State NMR Probe Components**. Jeffrey Dykstra, University of California, Irvine
B	407	**Molecular-level Insights into Biomineral Interfaces Revealed by Solid-state NMR**. Mounesha Garaga Nagendrachar, University of California San Diego
A	408	**Benchmarking DFT and Machine Learning for 19F NMR Crystallography**. Mohit Gupta, University of California Riverside
B	409	**Microwave Resonator for Nitrogen Vacancy Spin Control in High-Field NMR**. Himanshi Himanshi, University Of New Mexico
A	410	**Advanced DFT Models of ^{13}C Chemical Shift Tensors of Organic Crystals**. Robbie Iuliucci, Washington & Jefferson College
B	411	**Optical Detection of Nuclear Spin Ensembles in Diamond with NV centers**. Andrey Jarmola, UC Berkeley
A	412	**Structure of Isolated Yttrium Sites in Dealuminated Beta Zeolites**. Dulani Kumarasinghe, University of Virginia
B	413	**NMR-Assisted Crystallography of Aspartate Aminotransferase: Protonation States and Catalytic Mechanism**. Paula Magat, University of California, Riverside
A	414	**Tracking Electrolyte Decomposition and SEI Formation in Lithium ion Batteries Using Operando 19F NMR**. Emma Magee, McMaster University
B	415	**Fast and accurate NMR crystallography with Machine Learning Interatomic Potentials.** Frederic Mentink-Vigier, National High Magnetic Field Laboratory
A	416	**Structural Analysis of 13C and 15N Isotopically Labeled Chitin in its Natural Biological State via Solid-State NMR of Manduca sexta Pupal Cuticle**. William Nese, West Virginia University
B	417	**Solid-State NMR and DNP Investigation of PFAS Binding in Zr-Based MOFs**. Yifan Quan, University of Pennsylvania
A	418	**Triple-Resonance (HFX) Enables Separation of 19F-Mediated Cross-Relaxation Pathways under DNP**. Edvards Roberts Bensons, University of Rostock
B	419	**Determination of Atomically Precise Models of CdSe Quantum Dots Using DNP-Enhanced REDOR Solid-state NMR Spectroscopy**. Anuluxan Santhiran, Iowa State University
A	420	**Probing the Size Dependence of Knight Shifts in Doped Cadmium Oxide Nanocrystals Using 113Cd and 139La Solid-State NMR**. Robert Smith, Florida State University/National High Magnetic Field Lab
B	421	**Pushing the Limits: Resonance Assignment of a 144 kDa Enzyme via 1.1 GHz NMR**. Alexander Thome, University of California-Riverside
A	422	**Towards Microscale NMR at 14T using Quantum Diamond Sensors**. Chun Tung Cheung, University of Chicago
B	423	**Solid-State NMR to Elucidate Interactions of Small Molecule Fluorescent Dyes with Pathological Calcification Surfaces**. Sophie Young, University of California, San Diego

A	424	**Interpreting chemical shielding tensors: a well-posed approach through real-space analysis**. Josef Zwanziger, Dalhousie University
B	425	**1H led NMR Structure Determination in Molecular Solids**. Jacob Holmes, EPFL
A	426	**Structure Determination of 2D Germanane, Methyl Germanane and Methyl Germanane-Stannane Nanosheets by Nuclear Magnetic Resonance Spectroscopy**. Lukman Yunusa, Iowa State University
B	427	**Dynamic Nuclear Polarization with 1.3 mm Diameter Diamond Rotors**. Nicholas Wiesner, Massachusetts Institute of Technology
A	428	**Probing the limits to refocusing nuclear spin dynamics**. Chandrasekhar Ramanathan, Dartmouth College

101 **EPR Oral Session**

Optically induced spin polarization in open-shell molecular systems at variable magnetic fields

Ilya Dergachev, Yash Patel, Philip Weiss, Trent McHenry, Matthew Ross, Claudia E. Avalos*

Molecular Design Institute, New York University, New York, NY, 10003

The ability to optically initialize spin states has applications in sensitive magnetic field detection as well as magnetic resonance signal enhancement. Photoexcited triplet states in organic chromophores or defects in solids can be combined with microwave irradiation to significantly enhance NMR signals. Alternatively, in the absence of microwaves, the magnetic field can be tuned to specific matching conditions to allow for all optical nuclear spin polarization. One may also take advantage of nuclear spin-dependent relaxation pathways which are present in select molecular systems (Chemically induced dynamic nuclear polarization, or CIDNP). What all of these approaches have in common is that the electronic transition rates often determine the ultimate 'cooling power'. How polarized, or how intializable are these systems under the best conditions? What are the molecular motifs that would maximize the ground-state spin polarization in a subset of these systems and within a reasonable amount of time? In this presentation I will provide a broad overview of different classes of optically pumped molecular systems (their pros and cons), their dependence on magnetic field and I will discuss our recent efforts to determine which combination of molecular motifs lead to desirable electronic and magnetic coupling parameters to maximize multiplet and doublet electron spin polarization in chromophore-radical systems. We combine electronic structure calculations with experimental datasets and state-mixing dependent kinetic models to predict expected spin polarization in the excited and ground-state spin manifolds as a function of magnetic field.

Claudia Avalos - New York University
29 Washington Place New York, NY, 10003 United States, Email: claudia.avalos@nyu.edu

Spectroscopic and Theoretical Investigations of Co(II) and Fe(II) Compounds with a N_4S_2 Coordination

Sebastian A. Stoian,[1] Muhammad Zaeem Idrees,[1] Ronald Wright,[1] Kraig A. Wheeler,[2] Mikhaylo Ozerov,[3] Andrew Ozarowski,[3] Alina Dragulescu Andrasi,[1]

1. Department of Chemistry, University of Idaho, Moscow, ID 83844, USA
2. Department of Chemistry, Whitworth University, Spokane WA 99251, USA
3. National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA

High-spin cobalt(II) and iron(II) ions with a pseudo-octahedral geometry often exhibit large magnetic anisotropies. This behavior is caused by the spin-orbit coupling of the three lowest orbital states which have a T_{2g} parentage. Fine tuning the magnetic properties of these compounds is difficult and remains an important challenge in the quest for developing compounds with practical applications. Toward this aim we have synthesized two series of complexes supported by the tetradentate bpte = S,S'-bis(2- pyridylmethyl)-1,2-thioethane ligand. While the first series consists of mononuclear $Co^{II}(bpte)(NCX)_2$ complexes where NCX^- = $NCBH_3^-$, NCO^-, NCS^-, $NCSe^-$, the second series comprises three isostructural polymers of coordination $[M^{II}(bpte)(NC\text{-}N\text{-}CN)]ClO_{4¥}$ where M^{II} = Fe^{II}, Co^{II}, and Zn^{II}. The structures of these species were determined using single-crystal X-ray crystallography. The anisotropies of the cobalt(II) ions' ground Kramers doublets were assessed using high-frequency (HF) EPR and X-band EPR spectroscopies. The zero-field splitting of the ground spin quartet of these species was measured using Far-Infrared Magnetospectroscopy (FIRMS), magnetic susceptibility, and magnetization data. The zero-field splitting of the high-spin iron(II) sites was determined from a combined field-dependent ^{57}Fe Mössbauer and HF EPR study. In addition, the spin-crossover behavior of these species was probed using not only Mössbauer spectroscopy but also by magnetic susceptibility. The electronic structure of these complexes was investigated using *ab initio* CASSCF which allowed us to rationalize the spectroscopic data. We anticipated that the different energy gaps of the CN-based p_{HOMO}/p^*_{LUMO} orbitals of the NCX^- and $NC\text{-}N\text{-}CN^-$ coligands would allow us to control the crystal field splitting of the low-lying orbital states of the cobalt(II) and iron(II) sites. Our study revealed that while the choice of coligand affords some control over the magnetic anisotropy of the corresponding complex, there are additional factors that contribute to the magnetism of these species.

Sebastian Stoian - University of Idaho
875 Perimeter Dr, MS 2343 Moscow, Idaho, 83844 United States, Email: sstoian@uidaho.edu

Applied EPR for degradation mechanisms of per-and polyfluoroalkyl substances (PFAS): A scoping review

Isaac Spackman, Shubham Vyas

Colorado School of Mines, Department of Chemistry and Geochemistry, Golden, CO 80401

Adverse health effects due to exposure to per- and polyfluorinated 'forever chemicals' are estimated to cost more than $5 billion dollars yearly in the US alone, yet the cost to remove these persistent pollutants is estimated in *trillions* of dollars. Current remediation technologies are limited by both the costs of separation and primary energy costs resulting in few cases of economically viable scaling. These limitations have led to increased efforts to understand the fundamental chemical mechanisms at play in PFAS degradation to identify more energy efficient degradation strategies.

Many diverse decontamination strategies are thought to proceed through a series paramagnetic fluoroalkyl radical intermediates facilitated by reactive oxygen species or aqueous electrons, yet the fluoroalkyl radical intermediates common to these pathways have not been experimentally observed. The reason for this gap in evidence is currently unclear; the lifetimes of these intermediates are largely unknown and may not be sufficiently long to be observed via EPR. If the species are sufficiently long lived, rapid spin relaxation in the aqueous environment may also limit detection ability. Furthermore, commonly used experimental conditions and instrument settings might fundamentally preclude observation of these intermediates even if they were sufficiently long lived and had appropriate spin relaxation rates.

To clarify the extent of the evidence supporting such mechanisms, we present a scoping review focused on the use of EPR spectroscopy in PFAS degradation studies. Specifically, we aim to (1) describe the range of paramagnetic species that have been detected in PFAS degradation studies and (2) quantitatively evaluate the experimental conditions under which these species have been observed including pH ranges, reactant concentrations and critical spectrometer parameters. Finally, we present a qualitative analysis of the purpose and context in which EPR has been used for mechanistic studies of PFAS degradation, highlighting several ambiguities and misinterpretations in the literature.

Isaac Spackman - Colorado School of Mines
1500 Illinois St Golden, CO, 80401 United States, Email: ispackman@mines.edu

Very High Frequency (263 GHz) Pulse EPR Spectroscopy of High Spin Transition Metal Centers

Zikri Hasanbasri[1], Shasha Qiu[2], Guodong Rao[1], Amanda Caceres[1], Erica Debley[3], Pan Pan[4], Yuan Zheng[5], Ying Li[4], Jinjun Feng[4], Elizabeth M. Nolan[3], Marie Heffern[1], Paul Stucky[1], Neville C. Luhmann, Jr.[2], R. David Britt[1]

Department of Chemistry, University of California Davis, 1 Shields Ave, Davis, CA, 95616, USA. Department of Electrical and Computer Engineering, University of California Davis, 1 Shields Ave, Davis, CA, 95616, USA. Department of Chemistry, Massachusetts Institute of Technology, Cambridge MA, 02139, USA. National Key Laboratory of Science and Technology on Vacuum Electronics (NKLST-VE), Beijing Vacuum Electronics Research Institute (BVERI), Beijing, 100015,China. National Key Laboratory of Science and Technology on Vacuum Electronics (NKLST-VE), University of Electronic Science and Technology of China (UESTC), Chengdu, China.

Pulse Electron Paramagnetic Resonance (EPR) spectroscopy provides powerful tools for examining species with unpaired electrons, such as organic radicals and metal ions, in a wide variety of interesting systems. However, the lack of high-power pulse amplifiers at frequencies above 95 GHz has restricted their application at very high frequencies. Here, we showcase the development of a 10 W traveling-wave vacuum tube amplifier at 263 GHz, employed in a pulse EPR spectrometer. Pulse EPR at this high frequency is particularly useful for studying transition metals with S>1/2 that have large, broadening effects from "zero-field splitting" interactions, which often dominate the EPR spectra obtained at low frequencies. We show that the pulse EPR spectrometer at 263 GHz has a superb limit of detection, capable of resolving transition-metal impurities in a diamagnetic material. Furthermore, we highlight the resolution of the EPR spectra from a series of high-spin (S=5/2) Mn(II) complexes with metal sequestering proteins, in which the ZFS and the individual transitions are visibly differentiated.
Supported by NIH MIRA (R35GM126961) and DOE (DE-SC0025948 and DE-SC0007203).

Zikri Hasanbasri - University of California - Davis
141 Physical Sciences Mall, Chemistry Loading Dock Davis, California, 95616 United States, Email: zhasanbasri@ucdavis.edu

Room-Temperature Spin-Dependent Charge Carrier Transitions in Racemic and Chiral Polyacetylene $(CH)_x$ Thin-Film Diodes

C. Dhakal,[1] P. Poudel, R. M. Stolley[2], B. Odeke[1], N. C. Pak[1], J. S. Miller,[2] Z. V. Vardeny,[1] C. Boehme[1]

[1]*Department of Physics &; Astronomy, University of Utah, Salt Lake City, UT, USA*
[2]*Department of Chemistry, University of Utah, Salt Lake City, UT, USA*

Bipolar injection devices with an indium tin oxide (ITO)/Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS)/polyacetylene $(CH)_x$/Ca/Al architecture were fabricated using racemic, R-chiral, and S-chiral polyacetylene, synthesized via Shirakawa-type and BINOL-modified chiral catalyst systems. The devices exhibited reproducible rectifying current-voltage characteristics consistent with bipolar carrier injection and showed room-temperature continuous-wave electrically detected magnetic resonance (cw-EDMR), demonstrating the presence of spin-dependent electrical currents. CW-EDMR measurements performed at an excitation frequency of only 100 MHz indicate that the observed spin-dependent current is not driven by ensemble spin polarization but instead arises from spin-selection rules associated with the Pauli blockade. This interpretation is supported by the modulation-frequency dependence of the EDMR signal, which exhibits a maximum near 500 Hz and a sign reversal near 5 kHz, consistent with the dynamics of a coupled two-spin (S = 1/2) system. The cw-EDMR spectra revealed linewidths of approximately 9.5 G for racemic films and 7.5 G for both R- and S-chiral films. Differences between chiral and racemic devices were also observed for the bias dependencies of the EDMR signal strength, while the resonance conditions and line width of the observed EDMR signals remained nearly independent of the active layer material. Unlike the well-established spin-dependent polaron-pair recombination processes found in many p-conjugated polymers, the EDMR response in $(CH)_x$ occurs under both positive and negative bias conditions, suggesting that spin-dependent charge transport rather than recombination dominates the observed room-temperature EDMR response.

Chiranjibi Dhakal - University of Utah
270 S 1400 E Salt Lake City, UT, 84112 United States, Email: u1530930@utah.edu

Noninvasive EPR Detection of Melanin in Skin Melanomas: Why It Matters, How It Works, and What It Reveals

Mohammad Wehbi,[1*] Evelyne Harkemanne,[1,2*] Lionel Mignion,[3] Nicolas Joudiou,[3] Jean-François Baurain,[4] and Bernard Gallez.[1]

1. UCLouvain, Louvain Drug Research Institute, 1200 Brussels, Belgium
2. Dermatology Department, Cliniques universitaires Saint-Luc, 1200 Brussels, Belgium
3. Nuclear and Electron Spin Technologies, Louvain Drug Research Institute, 1200 Brussels, Belgium
4. Medical Oncology Department, Cliniques universitaires Saint-Luc, 1200 Brussels, Belgium
*. Equal contribution

Melanoma remains one of the most aggressive forms of skin cancer and is associated with reduced quality of life and survival at advanced stages. The development of a non-invasive, reliable, and early diagnostic method to confirm melanoma and estimate the depth of penetration in the skin (Breslow thickness) before surgery would enable clinicians to tailor therapeutic strategies from the outset and significantly shorten treatment delays. First, for patients with early-stage melanoma, immediate definitive surgical management could be performed with appropriate surgical margins. Second, for advanced melanoma, it would optimize the timing for initiating neoadjuvant immunotherapy. In this context, clinical low-frequency EPR, which characterizes melanin in superficial pigmented lesions, shows promise as an adjunct diagnostic method for melanoma. In this presentation, we will summarize 20 years of research[1-4] on this topic, emphasizing the challenges involved in detecting this endogenous free radical and the milestones that enabled the transition from *in vitro* samples to *in vivo* measurements in patients. We will also present the latest results from an ongoing clinical trial involving patients with suspicious lesions. At the time of writing this abstract, a first set of 141 lesions has been analyzed noninvasively in patients using multiharmonic clinical EPR. The EPR signal is significantly higher in melanoma than in benign atypical nevi (p < 0.0001). In addition, the EPR signal increases with the invasiveness of the lesion in the skin, with a significant difference observed between melanomas with high and low Breslow thickness (p < 0.001).

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Bernard Gallez - UCLouvain
Avenue Mounier 73.08, Louvain Drug Research Institute Brussels, Belgium, 1200 Belgium, Email: bernard.gallez@uclouvain.be

High Spatial Resolution Quantitative Oxygen Imaging Using Image Domain Averaging

Boris Epel[1,2], Irene Canavesi[1], and Mrignayani Kotecha[1]

[1] Oxygen Measurement Core, O2M Technologies, LLC, 2201 W Campbell Park Dr., Chicago, IL 60612, USA
[2]Department of Radiation and Cellular Oncology, The University of Chicago, Chicago, IL 60637, USA

Oxygen is central to metabolic activity, growth, reproduction, disease, and recovery pathways across all pathologies. Electron paramagnetic resonance oxygen imaging (EPROI) has emerged as the leading technique to image partial oxygen pressure (pO_2) maps in vitro and in vivo. The current gold standard for pO_2mapping using EPROI is inversion recovery electron spin echo (IRESE) with a radial acquisition scheme, which is fast, provides high pO_2 resolution, but suffers from lower spatial resolution. The other method, single point imaging (SPI), provides higher spatial resolution, but suffers from lower signal-to-noise ratio (SNR) and lower pO_2 resolution for T_2* imaging methodologies. In this work, we present advanced inversion recovery single point imaging (AIR-SPI) that overcomes the SNR limitations of SPI and provides T_1-based pO_2 maps with high pO_2 and high spatial resolution. In addition, AIR-SPI has lower power deposition due to being a free-induction decay (FID)-based method instead of an echo-based method. The AIR-SPI method is demonstrated in phantoms and mouse tumor images.

Boris Epel - O2M Technologies, LLC
2201 W Campbell Park Ave Chicago, IL, 60612 United States, Email: boris.epel@oxygenimaging.com

Noninvasive Assessment of Oxidative Stress in Normal and Diabetic Mice Wounds Using 1.0 GHz Rapid Scan EPR

Hanan Elajaili,[1] Tanden A. Hovey, [2] Nathan Dee,[1] Eva S. Nozik, [1] Sandra S. Eaton, [2] and Gareth R. Eaton[2]

[1]Cardiovascular Pulmonary Research Laboratories and Pediatric Critical Care Medicine, University of Colorado Anschutz Medical Campus, Aurora, CO 80045
[2]Department of Chemistry and Biochemistry, University of Denver, Denver, CO 80210

Oxidative stress and impaired redox regulation are key drivers of delayed wound healing, particularly in diabetes, yet direct spatially resolved assessment of reactive oxygen species (ROS) in vivo remains limited. Here, we evaluate oxidative stress in live mice using Rapid Scan EPR combined with redox-sensitive paramagnetic probes. Elevated ROS levels in diabetic mouse wounds were detected using 1 GHz Rapid Scan EPR spectroscopy and imaging[1] and a 10 mm surface coil.[2] Wild-type and db/db diabetic mice underwent cutaneous wounding and were administered the CMH (1-hydroxy-3-methoxy-carbonyl-2,2,5,5-tetramethylpyrrolidine) EPR imaging spin probe via subcutaneous injection at 3 days post-injury. Fifteen minutes following probe administration, wounds were examined in anesthetized mice. Spectral analysis revealed a composite signal arising from nitroxides with two distinct hyperfine constants (A_N = 16.0 G and A_N = 14.1 G), consistent with probes in aqueous and lipid microenvironments. The ratio of trapped radicals in non-polar to polar environments was higher in the diabetic mice, consistent with higher skin lipid content in obese diabetic mice. Two-dimensional spatial–spatial EPR images enabled visualization of probe distribution within mouse skin and wound tissue, demonstrating robust detection of ROS-related redox activity in vivo. Importantly, this approach enables noninvasive interrogation of ROS dysregulation associated with impaired diabetic wound healing. Future studies will employ a glutathione (GSH)-responsive probe to investigate thiol-mediated redox transformations and enable quantitative assessment of tissue GSH-dependent redox activity in skin and wound environments. Together, these results establish rapid scan EPR spectroscopy and imaging as powerful tools for characterization of environments for trapped radicals and for spatially resolved evaluation of oxidative stress and redox homeostasis in diabetic wound healing and related pathologies.

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Hanan Elajaili - University of Colorado Anschutz Medical Campus
12700 E9th Ave Aurora, CO, 80045 United States, Email: HANAN.ELAJAILI@CUANSCHUTZ.EDU

Ex Vivo Liver Electron Paramagnetic Resonance Oxygen Imaging for Optimization of Organ Preservation Time

Irene Canavesi[1], Casie Pandexter[2], Boris Epel[1,3], Basak E. Uygun[2], and Mrignayani Kotecha[1]

[1] Oxygen Measurement Core, O2M Technologies, LLC, 2201 W Campbell Park Dr., Chicago, IL 60612, USA
[2]Center for Engineering in Medicine and Surgery, Massachusetts General Hospital, Harvard Medical School, Boston, MA 02114, USA
[3]Department of Radiation and Cellular Oncology, The University of Chicago, Chicago, IL 60637, USA

Orthotopic organ transplantation remains the only viable method for treating end-stage organ diseases. Current preservation times for whole organs are limited to only a few hours of storage, resulting in inefficient use of available critical organs [1-3]. Since organ preservation is a multi-step process, potentially damaging to the organ, the non-invasive assessment for viability and function is important to optimize the preservation methods and increase the storage time. Trityl-OXO71-based electron paramagnetic resonance oxygen imaging (EPROI) is the only method that provides partial oxygen pressure (pO_2) maps that can be used to assess cell and organ viability [4,5]. In this study, ex vivo mouse liver pO_2 maps were acquired for three groups of livers (n = 4 each, 2 males and 2 females) in a petri dish: fresh, 48 hours post static cold storage (SCS) (48h-SCS), and 72 hours post SCS (72h-SCS). The pO_2 measurements were performed using the inversion recovery electron spin echo (IRESE) sequence[6]. The experiment included 90 minutes of continuous pO_2 imaging while perfusing the livers with 100% oxygenated media, 1 hour of warm ischemia (WI) period simulating the typical cutoff time for transplant organs, then another 90 minutes of pO_2 imaging again with perfusion of 100% oxygenated media to the livers. Mean pO_2 was calculated by masking the liver boundaries using the signal amplitude maps as well as pictures. A statistical difference between pre- and post-WI pO_2 was found for 48h-SCS and 72h-SCS groups (p-value < 0.0001), but not for fresh livers. A comparison between the three groups showed a statistical difference after WI between fresh-48h-SCS and fresh-72h-SCS, but not before WI, suggesting that livers from all groups were initially viable, but the 48h-SCS and 72h SCS groups did not survive the WI time. It was also found that more than 30% of voxels in the livers are hypoxic (pO_2 < 10 torr) in pre-WI time, indicating a high cellular oxygen consumption, but also exposure to hypoxic extracellular space. This is the first study, to the best of our knowledge, where EPROI is utilized to assess organ viability for transplantation.

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Irene Canavesi - O2M Technologies, LLC
2201 W Campbell Park Dr. Chicago, IL, 60612 United States, Email: irene@oxygenimaging.com

Impact of Heisenberg exchange on nitroxide T_1 in low viscosity solutions

Gareth R. Eaton and Sandra S. Eaton

Department of Chemistry and Biochemistry, University of Denver, Denver, CO 80210

The impact of Heisenberg exchange on nitroxide relaxation times is key to optimizing conditions for dynamic nuclear polarization (DNP). Although the impact on T_{2e} has been studied extensively, less data are available for T_{1e}. For low viscosity solutions Freed pointed out that nitroxide-nitroxide collisions have two potential outcomes. Collision with a nitroxide with a different nuclear spin (m_i) relieves saturation by moving the spin off resonance (Heisenberg exchange). Collision with a nitroxide with the same nuclear spin state has no impact on T_{1e}.[1] The effective spin lattice time constant observed in a CW power saturation experiment was shown to be the weighted average of the possible outcomes.[1]Pulse experiments have now been performed to separate these contributions to an inversion recovery curve from the two possible outcomes. For deoxygenated aqueous tempol solutions with concentrations between 0.015 and 5.9 mM, inversion recovery curves were fitted with a stretched exponential, the sum of two exponentials, and with a distribution of exponentials. These analysis methods show that there are two distinct contributions to the recovery curves. The concentration-dependent contribution is attributed to Heisenberg exchange, and the concentration-independent contribution is the 'true' T_{1e}.The ratios of the two populations are 2:1 for ^{14}N nitroxide and 1:1 for ^{15}N nitroxide, consistent with the statistical probabilities of collisions between radicals with the same or different nitrogen m_I.

Gareth Eaton - University of Denver
2101 E. Wesley Ave Denver, Colorado, Denver United States, Email: gareth.eaton@du.edu

Mechanism of CRISPR Target Discrimination Revealed by Site-Directed Spin Labeling

Peter Z. Qin

Department of Chemistry, University of Southern California, Los Angeles, CA 90089, USA

CRISPR (Clustered-Regularly-Interspaced-Short-Palindromic-Repeats) systems have been adapted into programmable agents for genome-wide manipulation of nucleic acids in many organisms, unleashing a revolution in genome editing and manipulation that is still rapidly advancing. Fundamental understanding on mechanisms of CRISPR target discrimination provides the foundation for CRISPR revolution, and is critical for overcoming remaining obstacles, such as the “off-target effects” that result in undersigned aberrant actions. Our group has been studying nucleic acids and protein-nucleic acid complexes using a unique biophysical technique, site-directed spin labeling, which monitors site-specifically attached stable radicals (e.g., nitroxide spin labels) using electron paramagnetic resonance (EPR) spectroscopy to gain structural (e.g., distance constraints) and dynamic (e.g., motions at the labeling site) information on the parent molecule under physiological conditions. Our current work centers on using site-directed spin-labeling in conjunction with other techniques to understand mechanisms of target discrimination by CRISPR-Cas9 and Cas12a that target double-stranded DNA. In this presentation, I will present work on applying the spin-labeling/EPR approach to reveal connections between effector conformational dynamics and DNA target discrimination by Cas9 and Cas12a.

Peter Qin - University of Southern California
Department of Chemistry, SGM 418, 3620 McClintock Avenue Los Angeles, CA, 90089 United States, Email: pzq@usc.edu

Order-of-Magnitude Sensitivity Gains in DEER via Dual-Mode PBG Resonators

Alex I. Smirnov, Sergey Milikisiyants, Antonin Marek, Hank Schmidt, Alexander A. Nevzorov

North Carolina State University, Department of Chemistry, Raleigh, NC, 27695-8204

Pulse EPR spectrometers at X- (9 GHz) and Q-band (35 GHz) typically employ cavity resonators to maximize sensitivity via strong microwave field confinement and efficient noise rejection achieved by resonant structures with high-to-moderate *Q*-factors. At W-band (95 GHz) and higher frequencies, non-resonant sample holders are more common, enabling broadband excitation via nanosecond pulses but at the expense of lower microwave field (B_1) amplitudes. This necessary trade-off between bandwidth, which is inversely proportional to *Q*, and achieving high B_1 field/noise rejection represents a critical limitation for double electron–electron resonance (DEER), where efficient spin manipulation at two distinct frequencies demands both wide bandwidth and high sensitivity for the detection of spin echoes after long delay times. Here we report on two advances for a fundamentally distinct class of EPR resonators based on one-dimensional photonic band gap (PBG) crystals. Firstly, we implement a PBG resonator architecture with continuously tunable external coupling, which allows for operating across undercoupled, critically coupled, and overcoupled regimes. Secondly, we introduce a dual-mode PBG resonator design in which the frequency separation between two high-*Q* modes is tunable up to 1.1 GHz, enabling optimization for DEER experiments. An oversized Q-band (34 GHz) PBG resonator constructed using a 3D-printed frame and a set of 2-inch sapphire discs achieved an unloaded quality factor of $Q \tilde{} 2.7\times10^4$ at room temperature under near-critical coupling conditions. Integration into a Bruker E580 spectrometer yielded at least an order-of-magnitude improvement in concentration sensitivity for echo-detected nitroxide signals. Comparable sensitivity enhancements were observed in dual-mode DEER measurements. These results demonstrate that the dual-mode PBG resonators can effectively mitigate the bandwidth–high *Q* trade-off, thus providing a scalable platform for high-sensitivity pulse EPR. Supported by NIH R01GM130821.

Alex Smirnov - North Carolina State University
2620 Yarbrough Drive, Campus Box 8204, , Cox Hall, Room 45, NCSU, Chemistry Raleigh, North Carolina, 27695-8204 United States, Email: aismirno@ncsu.edu

Navigating the Challenges of Excitation: Modeling Orientationally Selective Pulsed Dipolar EPR.

Nicholas A. Moriglioni,[1] Yannik Limbach,[2] Hassane El Mkami,[3] Katrin Ackermann,[2] Robert I. Hunter,[3] Graham M. Smith,[3] Bela E. Bode,[2] Sunil Saxena[1]

University of Pittsburgh, Department of Chemistry, Pittsburgh, PA 15260, U.S.A.University of St Andrews, School of Chemistry, St Andrews KY16 9ST, Scotland, U.K.SUPA, University of St Andrews, School of Physics and Astronomy, St Andrews KY16 9SS, U.K

Pulsed dipolar EPR spectroscopy has become a powerful tool for nanometer-scale distance measurements in biophysics. The combination of rigid spin labels, such as Cu(II)-NTA, with high-frequency EPR offers enhanced sensitivity and precise structural insight. However, these measurements are often limited by excitation bandwidth. With rigid spin labels, selective excitation may result in orientational selectivity, complicating data acquisition and analysis. As a remedy we have developed a model system which investigates acquisition schemes to obtain an orientationally averaged signal in as few experiments as possible. This method debuted in our work with DEER on the Cu(II)-NTA spin label at Q-Band.[1-3] Since then, we have developed the model to simulate both DEER and RIDME experiments at X-, Q-, and W-band. We've recently applied this model to find the optimal acquisition scheme for RIDME on Cu(II)-NTA at W-band (~95 GHz). We found that only four magnetic field positions are necessary to achieve an orientationally averaged signal despite excitation of only ~0.43% of the spin population. This framework provides an efficient means to overcome excitation limitations by finding optimal field positions informed by simulated PD-EPR. We expect the application of the model to be broadly applicable to high-field pulsed EPR studies with rigid spin labels. Supported by NSF BSF MCB 2407706.

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Nicholas Moriglioni - University of Pittsburgh
219 Parkman Ave. Pittsburgh, PA, 15213 United States, Email: nam253@pitt.edu

Quantum Spin Coherences in Photosynthetic Reaction Center Proteins

Jens Niklas, Jasleen K. Bindra, Yeonjun Jeong, Ahren W. Jasper, Lisa M. Utschig, Oleg G. Poluektov

Argonne National Laboratory, Chemical Sciences and Engineering Division, Lemont, IL 60439

Photosynthetic reaction center (RC) proteins are excellent model systems for studying the creation and control of coherent phenomena since they are well-defined, experimentally tunable systems. Following light-induced sequential electron transfer, photosynthetic RCs generate spin-correlated radical pairs (SCRPs), also referred to as spin qubit pairs (SQPs) in the field of quantum information science. Understanding and controlling coherence mechanisms in SQPs is important for realizing practical uses of electron spin qubits in quantum sensing applications. Here, we are using high-field/high-frequency electron paramagnetic resonance (EPR) spectroscopy at D-band (130 GHz, 4.6 T) to measure the coherence time of these SQPs in Photosystem I (PSI) and photosynthetic RC of purple bacteria (bRC) over a large temperature range. Deuteration of PSI showed negligible effect on the coherence time T_M, which is surprising, since nuclear spin diffusion involving protons was expected to be the main contributor to decoherence. While in the bRC deuteration led to a modest increase in T_M at low temperatures, the effect is still substantially smaller than predicted by classical nuclear spin diffusion. Computational modeling identified several methyl groups in the vicinity of the spin centers of both bRC and PSI, and methyl group tunneling at low temperatures has been previously suggested as a mechanism for enhanced spin decoherence. These results offer new insights for optimizing coherence times in quantum system design for quantum information science and sensing applications.

Jens Niklas - Argonne National Laboratory
9700 S. Cass Ave Lemont, Illinois, 60439 United States, Email: jniklas@anl.gov

X-band CW EPR Reveals Confined Water and Ice Embryos Inside AOT Reverse Micelles

John M. Franck[1], Romana Shathy[2], Alexandria Guinness[2]

ACERT, Ithaca, NY 14850Syracuse University, Department of Chemistry, Syracuse, NY 13244

X-band cw EPR is a suprisingly sensitive nanoscale viscometer. Here, nanoconfinement reshapes the dynamics and phase behavior of water itself, as observed inside the nanoscale water pool of AOT reverse micelles (RMs) from room temperature down to 230 K. We study two water loadings: w_0 = 3 (only unfreezable hydration water) and w_0 = 20 (includes free, freezable water). Spin probes in the water pool (TEMPO-sulfate) and at the surfactant interface (CAT-16) report Arrhenius activation energies for microviscosities[1]. Tighter confinement raises the activation energy for water viscosity (E_a = 31 vs. 17 kJ/mol for TEMPO-sulfate in w_0 = 3 vs. 20 RMs). Water in the interfacial layer requires 28 kJ/mol, regardless of RM size. This resembles NMR diffusivity measurements of small pores[2], but with 3D confinement, and goes one step further. Two dispersants are compared: dodecane, which freezes around the RMs, and isooctane, which remains liquid. Though calorimetry[3] shows no heat flow until “no-man’s land” (~ 230 K), the EPR spectra of RMs in dodecane exhibit two components in the supercooled regime that coexist over a range of at least 15 degrees. Specifically, three resolved hyperfine lines attest to mobile liquid water compartments in dynamic equilibrium with compartments that yield a slow-motional spectrum. The slow-motional component grows until dominating at the no-man’s land boundary, and reflects spin probes trapped with pre-critical ice embryos. In w_0 = 20 isooctane, the resolved lines instead broaden dramatically at a sharply defined temperature, slowly in time and without change in double-integrated intensity — a signature of embryos that grow into stable nuclei inside the RMs before exiting the RMs and sedimenting as bulk ice, progressively forcing the spin probe into smaller compartments. At w_0 = 3, neither dispersant produces an embryo signature. ESR thus directly probes pre-nucleation ice embryos in confined water.

John Franck - Advanced Center for ESR Research and Technology
206A Dryden Rd #107 Ithaca, NY, 14850 United States, Email: john.m.franck@acertcenter.org

Photogenerated spin polarization in quantum dot – molecule conjugates

Jacob Olshansky

Amherst College

Generating spin polarization is useful for both quantum computing and quantum sensing technologies. This talk will highlight a system that uses light to generate spin polarization in nanomaterials. A series of tunable quantum dot–organic molecule conjugates that can host photogenerated spin-based qubit pairs (SQPs) are presented. The photogenerated qubit pairs, composed of a spin-correlated radical pair (SCRP), are particularly intriguing since they can be initialized in well-defined, non-thermally populated, quantum states. The materials underlying this system are an organic molecular chromophore electron donor and a quantum dot acceptor composed of ZnO. A series of quantum dot–molecule conjugates are prepared that possess variable geometries. Photoexcited charge separation generates long-lived charge-separated radical pairs that are probed with light-induced time-resolved electron paramagnetic resonance (TR-EPR) spectroscopy. Notably, the EPR spectra of the radical pairs are dependent on the geometry of this highly tunable system. Overall, this work demonstrates the power of synthetic tunability in adjusting the spin specific addressability, satisfying a key requirement of functional qubit systems.

Jacob H. Olshansky - Amherst College
Amherst College Amherst, MA, 01002 United States, Email: jolshansky@amherst.edu

Understanding ESR-STM signatures of single spins at surfaces

Uwe Gerstmann and Katharina Lorena Franzke

Quantum Materials Modelling, Theoretical Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

The combination of electron spin resonance and scanning tunneling spectroscopy (ESR-STM) provides a new platform to access single spins of atoms and molecules on surfaces.[1,2] Characteristic hyperfine (hf) splittings can be measured and compared with theoretical predictions from density functional theory (DFT). In comparison with defects in bulk material, however, the calculated data deviates considerably from the experimental values. Limited accuracy of the exchange correlation functionals or the direct influence of the electric field of the STM-tip have been discussed as possible reasons. In this work, we show that the discrepancies stem from a relativistic effect, the suppression of orbital quenching at surfaces. In bulk material the influence of the ligand field ensures that the relativistic orbital contributions are cancelled out. As a consequence, over decades the restriction to isotropic Fermi-contact and anisotropic dipole-diploe interaction was very successful in semiconductors. Using a fully relativistic method we show that the assumption of orbital quenching is no longer valid at surfaces.[3] For Fe and Ti atoms on the MgO Ag(111) substrate, the spin-orbit driven effect improves the agreement with experimental ESR-STM data considerably, whereby the orbital contribution can be used as a direct measured for the suppression of orbital quenching. In accordance with previous assumptions,[4] we show that for Co on MgO/Ag(111) the magnetic anisotropic limit of 3d metal atoms is reached providing giant out-of-plane hf splittings in the 1.6 GHz regime.

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Uwe Gerstmann - Paderborn University
Warburger Straße 100 Paderborn, NRW, 33098 Germany, Email: uwe.gerstmann@upb.de

Probing Cu^2? Dopant Sites in Zn-based MOF-74 via EPR Spectroscopy

Pranjit Das[1], Andreas Pöppl[1*]

[1]Felix-Bloch-Institute of Solid-State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, Linnéstrasse 5, Leipzig 04103, Germany
Email: pranjit.das@uni-leipzig.de

Metal-organic frameworks (MOFs) continue to attract significant attention due to their tunable pore structures, chemical versatility, and potential applications in gas storage, catalysis, and separations [1–4]. Among these, MOF-74 (also known as CPO-27) is a widely studied framework for the study of dihydrogen isotope separation and storage because of the presence of open metal sites [5,6]. Introducing paramagnetic dopants like Cu^{2+} in MOF74 (Zn) facilitates the utilization of electron paramagnetic resonance spectroscopy (EPR), which is very sensitive to the local environment of the probe.

We investigated Cu^{2+}-doped MOF74 (Zn), using EPR to study the structural properties of the framework for utilization in the field of dihydrogen isotope storage and separation. Upon measuring with continuous wave EPR, it is evident from the EPR parameters that the Cu^{2+} species are incorporated in a distorted octahedral environment. Treating the as-synthesized sample with pulsed EPR techniques like 2pESEEM, 3pESEEM, and HYSCORE spectroscopy reveals further details about how the Cu^{2+} species is incorporated into the framework. It is evident that the Cu^{2+} species is incorporated at a Zn^{2+} framework site and binding to five oxygens from the framework and one solvent molecule. Upon activation, the solvent molecule gets removed, and the local environment of the Cu^{2+} species changes. The formation of such an open metal site is crucial for future dihydrogen separation and storage applications of this material. Further EPR will reveal the host-guest interaction of the framework and the hydrogen gas molecules.

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Pranjit Das - Leipzig University
Linnéstraße 5 Leipzig, Saxony, 04103 Germany, Email: pranjit.das@uni-leipzig.de

Organic Radical Dendrimers as Metal-Free T1 MRI Contrast Agents

Vega Lloveras,[1,2] Yufei Wu,[1] Chuanting Zhou,[1] Ehsan Shirdel,[1] Xuejiao Wang,[1] Songbai Zhang,[1] Luiz Pinto,[1] and José Vidal-Gancedo.[1,2]

1. Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), carrer dels Til.lers, 08193 Cerdanyola del Vallès, Spain
2. CIBER de Bioingeniería, Biomateriales y Nanomedicina, CIBER-BBN, 08913 Cerdanyola del Vallès, Spain.

Early detection of tumors is essential for improving patient survival, making magnetic resonance imaging (MRI) one of the most valuable tools for cancer diagnosis and monitoring. Although gadolinium-based contrast agents (GBCAs) remain the clinical standard for T1-weighted MRI, concerns regarding their toxicity have driven the development of safer, metal-free alternatives.
Persistent organic radicals are promising T1 contrast agents, but their clinical translation is hindered by low relaxivity and rapid bioreduction under physiological conditions. These limitations can be overcome by grafting multiple nitroxide radicals onto dendritic macromolecules, which enhance both relaxivity and radical stability through multivalency and steric shielding. Unlike conventional polymers, dendrimers offer well-defined architectures that enable precise control over radical number and spatial distribution.
Here, we report the synthesis of several generations of water-soluble radical dendrimers fully functionalized with peripheral nitroxide radicals.[1–4] Water solubility was achieved using either amino acid or PEG linkers, with amino acid-based dendrimers exhibiting superior performance.[4] EPR spectroscopy combined with molecular dynamics simulations revealed that radical location, water accessibility, and hydrogen-bonding interactions with nitroxide groups are key determinants of relaxivity.[3,4]
In vitro and *in vivo* MRI studies demonstrated that higher-generation radical dendrimers provide contrast enhancement comparable to, or greater than, commercial GBCAs.[1–4] In a murine GL261 glioblastoma model, they selectively accumulated in tumor tissue, enabling prolonged imaging (>2.5 h), while exhibiting high biological stability and renal clearance. These results highlight their potential as metal-free MRI contrast agents.

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Vega Lloveras - Institut de Ciència de Materials de Barcelona (ICMAB–CSIC)
Carrer dels Til.lers, 08193 Cerdanyola del Vallès, Spain Cerdanyola del Vallès, Barcelona, 08193 Spain, Email: vega@icmab.es

Decoherence of Nitroxide Spin Labels On Proteins

Samuel M. Jahn, Afrah Aftab, Rachelle K. Stowell, Maxx Tessmer, Stefan Stoll

Department of Chemistry, University of Washington, Seattle, WA, USA

Spin-labeling of proteins with nitroxide radicals is valuable both for characterizing protein conformational landscapes by EPR spectroscopy and for providing structurally precise scaffolds for potential spin qubit-based quantum sensing applications. At cryogenic temperatures, the phase memory times of nitroxide radicals, critical to both applications, are governed by the density and spatial distribution of nuclear spins, principally protons, within the unpaired electron's nanoenvironment. We employ an integrated computational approach combining protein structural modeling with spin dynamics simulations to predict nitroxide Hahn echo decoherence dynamics as a function of labeling site, with predictions that compare favorably against experimental data for maltose-binding protein. The spin dynamics simulations invoke an extended cluster correlation expansion (CCE) formalism that explicitly accounts for dynamic state-mixing effects arising from tunneling methyl groups on amino acid side chains. Finally, we demonstrate that phase memory times can be predicted semi-quantitatively from the structure of the spin-labeled protein alone without recourse to full quantum simulations via a simple empirical relation parameterized by local proton and methyl group counts.

Stefan Stoll - University of Washington
Box 351700 Seattle, WA, 98195 United States, Email: stst@uw.edu

Following Oxygen: Translational Advances in EPR Oximetry from Molecular Probes to Clinical Applications

Periannan Kuppusamy

Geisel School of Medicine, Dartmouth College, NH, USA

Oxygen plays a central role in physiology, pathology, and therapeutic response, particularly in cancer, cardiovascular disease, and radiation medicine. However, accurate and repeated measurements of tissue oxygenation in living systems have remained a longstanding challenge. Over several decades, advances in electron paramagnetic resonance (EPR) spectroscopy and imaging have enabled the development of technologies for direct and quantitative assessment of tissue oxygenation across biological scales. This lecture will present a perspective on the scientific journey and translational evolution of EPR-based oxygen sensing approaches, beginning with the development of oxygen-sensitive paramagnetic materials and in vivo EPR oximetry methods, followed by advances in imaging technologies and clinical translation.
The presentation will highlight key developments including the discovery and application of oxygen-sensitive crystalline probes, implantable oxygen sensors such as OxyChip, and recent efforts toward minimally invasive deep-tissue oxygen measurements using OxyTrack technology. Studies demonstrating applications in tumor hypoxia, radiation response, and hyperoxic interventions will be discussed. In addition, recent efforts integrating EPR oximetry with oxygen-enhanced MRI for quantitative oxygen mapping (qOE-MRI) will be presented as a framework for combining direct oxygen measurements with high-resolution imaging. Collectively, these studies illustrate the progression of EPR from a powerful spectroscopic tool to a clinically relevant technology for precision medicine. Future opportunities and remaining challenges for quantitative oxygen assessment in biomedical research and patient care will also be discussed.

Periannan Kuppusamy - Geisel School of Medicine at Dartmouth College
1 Medical Center Drive, Bldg Rubin, Room 601 Lebanon, NH, 03756 United States, Email: Periannan.Kuppusamy@Dartmouth.edu

Insights into Second-Shell Waters of Gadolinium Contrast Agents using Electron-Nuclear Double Resonance (ENDOR): Implications for Relaxivity and Dynamic Nuclear Polarization

Martyna Judd,[1] Peter E. Doan,[1] Matthew D. Bailey,[1] Thomas J. Meade,[1] Brian M. Hoffman,[1] Songi Han.[1]

[1]Northwestern University, Department of Chemistry, Evanston, IL, 60208, USA

Water molecules in the second coordination sphere of Gd^{3+} contrast agents modulate proton relaxivity.[1] However, their organization, dynamics, and quantitative contribution remain poorly constrained and difficult to untangle from inner- and outer-sphere water dynamics. Conventional relaxometry approaches e.g. nuclear magnetic relaxation dispersion, rely on model-dependent interpretations[1,2] that can become murky when contending with heterogeneous or transient hydration environments. Hence, key parameters governing water exchange, hydrogen-bonding networks, and outer-sphere contributions remain difficult to validate experimentally. Electron paramagnetic resonance (EPR) methods are typically used to constrain the contributions of paramagnetic rotational correlation and spin-lattice relaxation times to the overall water relaxivity mechanism.[2,3] Here, we extend EPR methods to investigate second-shell water interactions in Gd^{3+} complexes, using ^{1}H and ^{2}H electron–nuclear double resonance (ENDOR) spectroscopy at 2 K. ENDOR directly probes the hyperfine coupling distribution in the sample, and therefore the distribution of coordination dynamics. Additionally, by detecting only on the |-7/2> to |-5/2> Gd^{3+} transition we can probe first vs. second-shell water populations in isolation, allowing their spatial and dynamic characteristics to be distinguished. Finally, we explore how the tethering of Gd^{3+} contrast agents to nanodiamond surfaces – which has been shown to give 10-fold relaxivity enhancement[4] – impacts the hydration shell. Critically, there is limited understanding behind this enhancement and whether water confinement and surface interactions play a role. We use ENDOR to model the hydration dynamics in these systems, and additionally explore the potential of resonance matching between nanodiamond P1-centers and Gd^{3+} as a way to enhance dynamic nuclear polarization efficiency at ambient temperature.

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Martyna Judd - Northwestern University
2170 Campus Drive, Silverman 4560 Evanston, IL, 60208 United States, Email: martyna.judd@northwestern.edu

Room-temperature hyperpolarization and its applications in quantum sensing

K. Tateishi[1,2,3]

1. Nishina Center for Accelerator-Based Science, RIKEN, Saitama 351-0198, Japan
2. Pioneering Research Institute, RIKEN, Saitama 351-0198, Japan
3. Institute for Quantum Life Science, National Institutes for Quantum Science and Technology (QST), Chiba 263-8555, Japan

I present a room-temperature hyperpolarization technique based on dynamic nuclear polarization using photoexcited triplet electrons (triplet-DNP) that operates efficiently under low magnetic fields. By exploiting the photoexcited triplet states of pentacene as a polarizing agent, we achieve proton polarization exceeding 60% at 0.65 T and room temperature.[1] This represents a significant advance over conventional DNP approaches, which typically require cryogenics and a superconducting magnet.

The ability to generate high nuclear spin polarization under mild conditions enables practical and scalable quantum sensing. One key application is DNP-enhanced magnetic resonance imaging (DNP-MRI), where signal enhancement allows highly sensitive, non-invasive probing of biological systems. This approach enables real-time sensing of physiological environments, with the potential to detect subtle metabolic or microenvironmental changes in living organisms. In addition, our hyperpolarization system can be applied as a "polarized target" for nuclear physics experiments.[2] Both low-field and room-temperature operation have advantages in minimizing perturbations to charged particle trajectories and suppressing radiation damage. This improves the flexibility of studies of nuclear forces and internal nuclear structure.

Overall, these results demonstrate that triplet-DNP provides a versatile route toward high-efficiency hyperpolarization under practical conditions, bridging quantum sensing applications, including biomedical imaging and nuclear physics research.

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Kenichiro Tateishi - RIKEN
2-1, Hirosawa Wako, Saitama, 351-0198 Japan, Email: kenichiro.tateishi@riken.jp

Registered EPROI And Ultrasound Imaging for Monitoring Tumor Oxygenation and Therapy Response

Gabriela Dziurman[1,2], Natalia Radzikowska[1], Aleksandra Murzyn[1,2], Piotr Swierzewski[1,2], Agnieszka Drzal[1], Malgorzata Szczygiel[1], Martyna Krzykawska-Serda[1], Martyna Elas[1]

[1]Jagiellonian University, Faculty of Biochemistry, Biophysics and Biotechnology, Department of Biophysics and Cancer Biology, Krakow, Poland
[2]Jagiellonian University, Doctoral School of Exact and Natural Sciences Faculty of Biochemistry, Biophysics and Biotechnology, Department of Biophysics and Cancer Biology, Krakow, Poland

Tumor oxygenation is a dynamic component of the tumor microenvironment and may influence therapeutic efficacy. In this study, we aimed to investigate changes in tumor pO_2 before and after treatment with X-ray irradiation and salinomycin, and to determine whether oxygenation dynamics is associated with tumor response. In vivo electron paramagnetic resonance oxygen imaging (EPROI) was combined with ultrasound-based anatomical imaging (B-mode), allowing registration of functional pO_2 maps with tumor morphology. Measurements were performed before therapy and at selected time points after treatment. Oxygen-sensitive probe OX071 was administered intravenously or intraperitoneally in order to compare delivery routes and evaluate differences in signal kinetics and spatial information.
The main experimental output consisted of longitudinal images showing tumor oxygenation before and after therapy. Registered EPR and ultrasound images enabled visualization of heterogeneous pO_2 distributions within the tumor volume and their therapy-induced modulation[1]. Images obtained after intraperitoneal probe administration demonstrated that this route is feasible for EPR oxygen imaging [2], although the observed kinetics differed from intravenous administration. These differences suggest that IV and IP delivery may provide complementary information about probe distribution, accessibility of the tumor microenvironment, and the temporal window suitable for imaging. Histological analysis was used to support the imaging results and to assess treatment-related alterations in tumor architecture
Our results demonstrate that EPROI can detect changes in tumor pO_2 induced by X-ray irradiation and salinomycin treatment. These pO_2 changes may be related to tumor response, as has been shown in histological data. The registration of oxygen maps with US imaging provides anatomical interpretation of oxygen maps. Both intravenous and intraperitoneal probe administration are applicable, but their distinct kinetics require further investigation to optimize imaging protocols and biological interpretation.
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Gabriela Dziurman - Jagiellonian University
Krakow, Gronostajowa 7 Krakow, malopolska, 30-387 Poland, Email: gabriela.dziurman@uj.edu.pl

Characterization of the Cu(II)-NTA spin label on proteins by x-ray crystallography and electron paramagnetic resonance

Jessica E. Besaw,[1] Jörg Reichenwallner,[1] Julia S. Barbat,[2] D. Darya Porat,[3] Arne Reuter,[4] Tobias Hett,[4] Olav Schiemann,[4] Oliver P. Ernst,[1,2,3]

1. University of Toronto, Department of Biochemistry, Toronto, ON M5S 1A8, Canada
2. University of Toronto, Department of Materials Science and Engineering, Toronto, ON M5S 1A8, Canada
3. University of Toronto, Department of Molecular Genetics, Toronto, ON M5S 1A8, Canada
4. University of Bonn, Clausius-Institute for Physical and Theoretical Chemistry, 53115 Bonn, Germany.

Site-directed Cu(II)-labelling in pulsed electron paramagnetic resonance (EPR) spectroscopy has demonstrated narrow Cu(II)-Cu(II) distance distributions suitable to resolve subtle protein conformational changes. The high precision derives from a double histidine (dHis) mutation that effectively locks a Cu(II)-nitrilotriacetic acid (Cu(II)-NTA) moiety in place. Prior to this work, no structures featuring the dHis-Cu(II)-NTA motif had been resolved [1]. This talk presents numerous atomic-resolution crystal structures of the dHis-Cu(II)-NTA label on the a-helices of T4 Lysozyme (T4L) and the ß-sheets of mScarlet3 [1-3]. Our research captured the rigid octahedral coordination of the dHis-Cu(II)-NTA complex. We link these rigid binding modes to their low micromolar binding affinities and narrow Cu(II)–Cu(II) distance distributions. We additionally expanded the application of dHis-Cu(II)-NTA labelling to loop-based protein structural elements. Using T4L as the model protein, we identified dHis loop variants that effectively chelate Cu(II)-NTA with high affinity, exhibit well-defined coordination geometry, and give narrow Cu(II)–Cu(II) distance distributions in pulsed EPR studies. This research provides guidelines to improve dHis site-selection and offers geometric constraints that can be leveraged in modeling and molecular dynamics programs to extract protein structural details from EPR experiments.

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Oliver Ernst - University of Toronto
1 King's College Circle Toronto, Ontario, M5S1A8 Canada, Email: oliver.ernst@utoronto.ca

Electrostatic Environment in Phospholipid Vesicles: Layer by Layer, Inside and Out

Ngan Nguyen, Maxim A. Voinov, Alex I. Smirnov, Tatyana I. Smirnova

North Carolina State University, Raleigh, NC

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. One method for assessing surface electrostatics involves determining the pK_a shift of protonatable molecular probes. Previously, we successfully employed EPR of phospholipids labeled at the headgroup with a pH-sensitive nitroxide to map bilayer interfacial electrostatics. Here, we report on a comparative study of the surface electrostatics of multilamellar (MLVs) and unilamellar vesicles (ULVs) composed of either POPG or POPC lipids. For vesicles composed of negatively charged POPG, the effective pK_a measured for MLVs was significantly, up to 0.9 pH unit, higher than that for ULVs across all three probes. The larger local electrostatic potential experienced by probes within the inner lamellae is likely due to an influence of charges on the adjacent lamellae. For zwitterionic POPC, the effective pK_a for MLVs was only slightly lower than that for ULVs, suggesting that the electrostatic environment in the inner lamellae closely resembles that of the outermost and innermost layers, with minor differences potentially arising from variations in hydration and ion distribution. We then measured the protonation state of probes at the surfaces of outer or inner leaflets of DMPG ULVs and observed a significant shift in pKa, indicating a difference in electrostatic or local dielectric environments of the probes. The results further highlight the utility of the spin-labeled phospholipids in biophysical EPR spectroscopy and reveal unexpectedly large changes in layer-dependent electrostatic environments in MLVs and ULVs. This material is based upon work supported by the National Science Foundation under Grant No. 2305172.

Tatyana Smirnova - North Carolina State University
2620 Yarbrough Dr, NCSU Raleigh, NC, 27695 United States, Email: tismirno@ncsu.edu

Applications of EPR to Biopharma: Structure, Dynamics, and Equilibria of a Monomer-Dimer System by Pulsed Dipolar Spectroscopy

Austin R. Gamble Jarvi[1]

High Q Technologies, Waterloo, ON, Canada

Pulsed Dipolar Spectroscopy (PDS), a branch of Electron Paramagnetic Resonance (EPR) spectroscopy that focuses on the measurement of interspin dipolar interactions, holds significant value for the investigation of protein-protein interactions (PPIs), capable of elucidating structural constraints, determining dynamic information, and counting coupled spins. Protein oligomerization is a specific type of PPI of great interest to pharmaceutical and drug-discovery industries. Because oligomerization influences and regulates many key protein categories such as enzymes, ion channels, and transcription factors, it plays a vital role in many biological and physiological processes that make appealing targets for therapeutic development. Therefore, understanding the mechanism of interaction is of significant interest to the scientific community.

Here, we apply Double Electron Electron Resonance (DEER), a robust and popular PDS technique, to investigate the dimerization of a homodimeric protein system. The distance distributions extracted from the DEER data are used to gain insight into the structure and dynamics of the dimeric complex, while careful analysis of the modulation depth of the dipolar traces reveals the populations of monomer and dimer states. Furthermore, we investigate the changes in these aspects as a function of buffer conditions and against the introduction of compounds that promote dimerization of the protein. These findings exemplify the capacity of EPR to contribute to questions across the PPI space, and the principles demonstrated here can be easily extrapolated toward other hot-topics within the biopharmaceutical industry, such as induced proximity and targeted protein degradation.

Austin Gamble Jarvi - High Q Technologies
485 Wes Graham Way Waterloo, Ontario, N2L0A7 Canada, Email: austin.gamblejarvi@highqtechnologies.com

Atomistic pictures of slow protein conformational changes using EPR and simulations.

Shramana Palit, Darian T. Yang, Xiaowei Bogetti, Anthony Bogetti, Olivia Wood, Lillian T. Chong*, and Sunil Saxena*.

Department of Chemistry, University of Pittsburgh, Pittsburgh PA 15260, USA

Large-amplitude protein conformational changes are central to many cellular processes. However, capturing the pathways of these changes remains an extant challenge. Electron paramagnetic resonance (EPR) spectroscopy can report on these changes through distance measurements between site-directed spin labels, but does not provide atomistic resolution. Conversely, conventional molecular dynamics (MD) simulations offer detailed structural insight but often fail to access the long timescales over which such transitions occur.
In this work, we integrate weighted ensemble (WE) path sampling with EPR-measured distance restraints to directly capture the transition pathways between conformational states of lysine/arginine/ornithine binding protein (LAOBP). Using this approach, we generated hundreds of trajectories that describe the large-scale transition between the closed (ligand-bound) and open (ligand-free) states. Analysis of these pathways revealed key residue-level interactions that govern the transition. Guided by these insights, we performed selected mutagenesis that stabilized the protein in its open state. Together, these combined techniques allow the visualization of hidden alternate states while also providing a mechanistic understanding that guides the rational tuning of protein function.1

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Shramana Palit - University of Pittsburgh
219 Parkman Ave Pittsburgh, PA, 15260 United States, Email: shp176@pitt.edu

Direct Detection of Multiple Distance Peaks from Pulsed Dipolar Signals

Utkarsh Misra[1,3], Shikhar Prakash[1], Aritro Sinha Roy[2,3], Jack H Freed[2,3], Madhur Srivastava[2,3,4,*]

[1] Department of Systems Engineering, Cornell University, Ithaca, NY 14850, United States
[2] Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, 14850, United States.
[3] National Biomedical Resource for Advanced ESR Spectroscopy, Cornell University, Ithaca, NY 14853 USA.
[4] Cornell Atkinson Center for Sustainability, Cornell University.

Here, we introduce an independent comparison framework for pulsed dipolar electron spin resonance. Recovering distance distributions P(r) from PDS time-domain signals is an ill-posed inverse problem, and samples with different underlying distance distributions can sometimes produce nearly indistinguishable time-domain signals, making it useful to have an additional way to confirm whether two samples truly differ in conformation. The framework quantifies differences in the underlying distance distributions directly from PDS signals, without relying solely on full distribution reconstruction.
The resulting dissimilarity metric offers several advantages: (1) it reliably determines the number of peaks present in a distribution; (2) it distinguishes two closely spaced peaks from a single broader peak once their separation exceeds 1 Å; (3) it recovers peak positions and mixture compositions in overlapping distributions and (4) it correlates systematically with differences in the distance distributions. All while remaining consistent with results from established reconstruction methods.
The framework leverages a time-frequency domain representation of PDS signals to enable this direct, quantitative comparison. Signals are transformed using continuous wavelet transforms and compared using the structural similarity index measure (SSIM). We validate this approach on simulated distance distributions as well as experimental data from rigid biradicals and SOD1 mutants linked to amyotrophic lateral sclerosis (ALS), where the results closely match those obtained from established methods.
This time-frequency comparison framework offers a complementary, reconstruction-independent strategy for confirming differences in distance distributions between PDS samples, with particular value for distinguishing closely related or highly overlapping conformational states in proteins.

Utkarsh Misra - Cornell University
116, Thurston Avenue Ithaca, New York, 14850 United States, Email: um48@cornell.edu

A Modular Low-Power 329 GHz Platform for Integrated EPR, NMR, and DNP

O. Laguta[1], J. Dubský[1], P. Drexler[2], P. Neugebauer[1]

1. Brno University of Technology, Central European Institute of Technology, Brno, 61200 Czech Republic
2. Brno University of Technology, Faculty of Electrical Engineering and Communication, Brno, 61200, Czech Republic

Dynamic nuclear polarization is conventionally implemented using high-power microwave irradiation, typically generated by gyrotrons[1,2], to achieve substantial nuclear spin hyperpolarization. While effective, such systems are complex, costly, and energy intensive. Here, we present an alternative DNP approach based on a low-power, solid-state microwave source delivering 60 mW at 329 GHz. The system is built around a multifunctional probe that allows for EPR, NMR and DNP experiments within a single platform. This is especially useful for EPR studies of polarizing agents in the same magnetic field as used in the DNP experiments. The probe follows a modular design in which the NMR module (rf coil and associated electronics) is interchangeable, allowing straightforward adaptation to different nuclei. The system is coupled to a Bruker Avance NEO 500 MHz NMR spectrometer and uses standard EPR and NMR tubes with sample volume up to 100 uL, ensuring compatibility with standard high-resolution NMR workflows. Despite the significantly lower microwave power compared to gyrotron-based systems, the setup demonstrates robust DNP performance. We observe an enhancement factor of approximately 10 for ^{31}P NMR signals in triphenylphosphine with BDPA as a polarizing agent, and for ^{13}C nuclei in microdiamond samples, signal enhancements exceed 1000. These results demonstrate that substantial DNP enhancements can be obtained using compact, low-power microwave technology and it opens new possibilities for broader adoption of DNP-enhanced spectroscopy in laboratories with limited infrastructure.
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Oleksii Laguta - Brno University of Technology
Purkynova 123 Brno, Southmoravian, 612 00 Czech Republic, Email: oleksii.laguta@ceitec.vutbr.cz

Recent advances in EPR cryoprobes

Vidmantas Kalendra[1], Gediminas Usevicius[1], Ignas Pocius[1], Justinas Turcak[1], Uršule? Tarvydyte?[1], Juras Banys[1], John J.L. Morton[2,3] and Mantas Šimenas[1]

1. Faculty of Physics, Vilnius University, Sauletekio 3, LT-10257, Vilnius, Lithuania
2. London Centre for Nanotechnology, University College London, London WC1H 0AH, UK
3. Department of Electronic &; Electrical Engineering, University College London, London WC1E 7JE, UK

Inspired by the success of NMR cryoprobes, we recently reported a leap in EPR sensitivity by equipping ordinary X- and Q-band EPR probeheads with a cryogenic low-noise microwave amplifiers placed close to the sample.[1,2] The reported probeheads support high-power pulsed EPR experiments and are compatible with standard EPR resonators and samples. Here, we discuss recent advances in the field concentrating on the switch-based cryoprobe designs[3] and other strategies to approach sensitivity limits of EPR cryoprobes.

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Mantas Simenas - Vilnius University
Sauletekio av. 9 Vilnius, Vilnius, 10222 Lithuania, Email: mantas.simenas@ff.vu.lt

Improving the modulation in 4-pulse DEER with swept observer pulses

Eric R. Lowe[1], Stefan Stoll[2], Jason P. Kestner[1]

University of Maryland Baltimore County, Department of Physics, Baltimore, MD 21250University of Washington, Department of Chemistry, Seattle, WA 98195

Swept pump pulses are known to improve DEER modulation depth by exciting a larger fraction of the spin label spectrum.[1] Here we extend the idea to the observer side, replacing the narrowband observer pulses of the 4-pulse DEER sequence with frequency-swept pulses, using a composite pulse sequence to prevent phase dispersion. Optimal pulse shapes for the swept observer pulse sequence are obtained by numerical maximization of the modulation-to-noise ratio (MNR), explicitly accounting for the microwave resonator transfer function and microwave power limitations. We benchmark the new approach for nitroxide-nitroxide and Cu(II)-Cu(II) DEER against Gaussian observer pulses, with both pulse shapes optimized under the same constraints. We find that the improvement for nitroxides is marginal. However, for the much broader Cu(II) spectrum, we see a 45% improvement in MNR, indicating that swept observer excitation is most beneficial for broadband spectra.

Eric Lowe - University of Maryland, Baltimore County
7830 Paragon Circle, Apt 411 Elkridge, Maryland, 21075 United States, Email: elowe2@umbc.edu

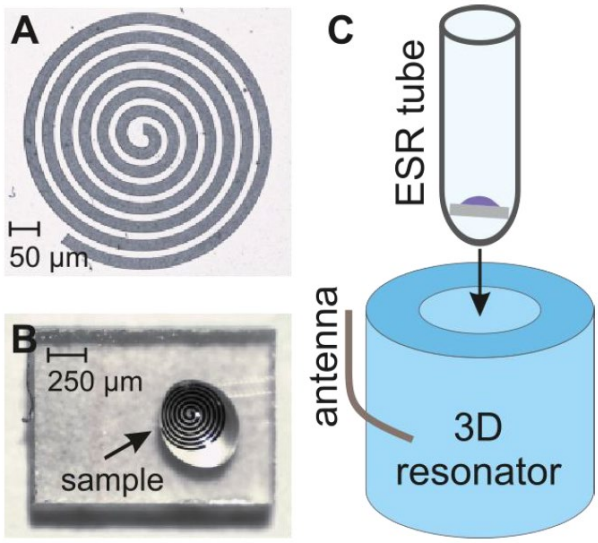
Versatile High-Sensitivity EPR Using Superconducting Spiral Microresonators

G. Usevicius[1], O. W. Kennedy[2], I. Pocius[1], P. Hogan[2], A. V. R. de Temino[2], J.-B. Verstraete[2], G. A. Jacob[2], J. Alexander[2], V. Kalendra[1], J. Banys[1], John J.L. Morton[2,3], M. Šimenas[1]

[1]Faculty of Physics, Vilnius, University, Sauletekio av. 3, LT-10257 Vilnius, Lithuania
[2]London Centre for Nanotechnology, University College , London WC1H 0AH, UK
[3]Dept. of Electronic &; Electrical Engineering, University College London, London WC1E 7JE, UK

Electron spin resonance (EPR) is a versatile technique widely applied in structural biology, quantum information science, solid-state physics, and chemistry. However, conventional EPR setups typically require microliter-to-milliliter sample volumes to achieve adequate signal-to-noise ratios, which restricts investigations of volume-limited systems. Enhancing spin sensitivity while maintaining compatibility with standard laboratory instrumentation remains a key challenge.

In this work, we present a planar microresonators fabricated from high-temperature yttrium barium copper oxide (YBCO) superconductor, designed for operation at both X- and Q-band frequencies (9.5 and 34 GHz). The device employs a spiral geometry that, at X-band, supports a microwave mode volume of approximately 7 nL. To facilitate practical implementation, we introduce a coupling scheme in which the planar microresonator is integrated into a conventional 3D EPR cavity. This design preserves compatibility with existing instrumentation while enabling operation at magnetic fields above 1 T and temperatures up to 80 K under standard conditions. The performance of the superconducting spiral microresonator is demonstrated through pulsed EPR measurements on representative systems, including DEER, ESEEM, and ENDOR experiments.



Gediminas Usevičius - Vilnius University
Sauletekio av. 3 Vilnius, Vilnius, 10222 Lithuania, Email: gediminas.usevicius@ff.vu.lt

Microresonators for Small Volume X-band EPR Measurements of Aqueous Protein Samples

Anand Anilkumar,[1] and Jason W. Sidabras[1]

1 Medical College of Wisconsin, Department of Biophysics, Milwaukee, WI 53226

Commercially available EPR cavity resonators typically require sample volumes on the order of tens to hundreds of microliters of sample, to record a spectrum with sufficient SNR. This is not ideal for biological studies involving volume-limited protein samples, particularly proteins with lower expression levels, or proteins that are difficult to purify. The microspiral resonator, fabricated by rolling a 10 µm copper sheet to a spiral structure (Figure (A)-(C)), is a promising alternative due to its exceptionally small sample volume (100 - 400 nL), improved EPR sensitivity, and favorable microwave field distribution for aqueous protein samples. The spiral architecture generates a homogeneous magnetic field along the sample region, while the electric field is confined between the spiral turns (Figure (D) and (E) respectively). This spatially separated electromagnetic field distribution reduces the electric field associated aqueous losses, and improves the filling factor, making the microspirals well suited for volume-limited protein samples. Here we report the simulation, and fabrication of microspiral resonators designed for X-band EPR measurements of small volume aqueous protein samples.

The sensitivity of the resonator was assessed by calculating signal values at constant B_1 using ANSYS HFSS eigenmode simulations of a copper microspiral with a 0.35 mm O.D and 0.2 mm I.D glass capillary tube holding 240 nL water (Figure (A) and (B)). The signal values were compared against a TE_{01d} Sapphire dielectric resonator with the same sample volume. The simulations revealed a twofold improvement compared to the dielectric resonator, directing advancements in concentration sensitivity. Microspirals were fabricated by rolling copper sheets by hand based on the number of turns and spiral length determined from the simulations. The fabricated spirals were characterized using a VNA revealing Q-values of 100 - 200 with the sample, which are suitable for aqueous EPR measurements. The Q-values are maintained due to the efficient confinement of the microwave electric field and minimum overlap with the aqueous sample.

The simulated twofold signal improvement, nanoliter-scale active volume, high filling factor and improved magnetic field distribution leads to the capability of microspiral resonators for low-volume EPR measurements. By integrating the microspiral with 3D printed microfluidic devices and flow control systems, volume limited aqueous protein samples can be precisely delivered to the resonator sample region. The platform is expected to improve SNR, enable integration with microfluidic devices, and enable advanced EPR measurements, including Saturation Transfer EPR for volume-limited aqueous protein samples. Overall, this work establishes an instrumentation framework for lab-on-a-chip EPR platforms with precise sample handling and enhanced EPR sensitivity for biological applications.

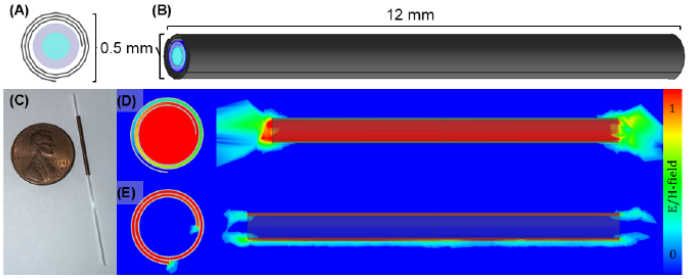


Figure: (A) Cross sectional and (B) Side view of copper microspiral made by rolling 10 μm copper sheet to 2.5 turns with an I.D of 0.4 mm and O.D of 0.5 mm with glass capillary sample tube, (C) Fabricated copper microspiral with the sample tube. Normalized (D) Magnetic and (E) Electric field distribution inside the spiral.

Anand Anilkumar - Medical College of Wisconsin
8701 Watertown Plank Rd. Milwaukee, WI 53226 Milwaukee, WI, 53226 United States, Email: aanilkumar@mcw.edu

Operando Monitoring of the Growth of Lithium Metal Dendrites Using EPR-on-a-Chip (EPRoC)

Matan Perez[1], Annica Freytag[2], Michal Kern[3], Jens Anders[3], Pedro Groszewicz[1], Klaus Lips[1,4,5]

[1]Department of Spins in Energy Conversion and Quantum Information Science (ASPIN), Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany
[2]Department of Chemistry, Humboldt University of Berlin, Berlin, Germany
[3]Institute of Smart Sensors, University of Stuttgart, Stuttgart, Germany
[4]Department of Physics, Freie Universität Berlin, Berlin Germany
[5]Department of Physics and Astronomy, University of Utah, Salt Lake City, USA

Batteries based on lithium metal anodes offer a significantly higher specific capacity when compared to graphite anodes currently used in lithium-ion batteries. However, lithium metal exhibits inhomogeneous plating during charging that leads to the growth of microstructures (e.g. dendrites), causing short-circuits and preventing its commercial use. Characterization methods with high sensitivity to lithium metal are essential in understanding growth mechanisms and develop mitigation strategies. Electron paramagnetic resonance (EPR) spectroscopy can monitor lithium dendrites, yet conventional cavity-resonator systems cannot selectively probe the deposited lithium, which is convoluted with the bulk lithium signal from the counter electrode. Here, we introduce an EPR-on-a-chip (EPRoC) approach that allows the use of simple electrochemical cells and restricts the sensing volume to plated lithium on the negative electrode, greatly simplifying spectral interpretation and enabling detection of the early onset of lithium plating. Using a physical model for conduction EPR (CEPR), the operando EPRoC signal of lithium plating on copper is utilized as a surrogate for anode-less batteries, enabling identification of charging stages associated with dendritic growth. Combined with a thin-film CEPR approximation and a triple-phase stochastic model optimized via deep learning, our approach maps signals to dendritic growth characteristics and provides new insight into lithium deposition behavior. In addition, we show that magnetic field distortions within lithium, induced by morphology-dependent paramagnetic susceptibility gradients induced by the solid-electrolyte interphase (SEI), lead to a Gaussian distortion of the CEPR line shape. This facilitates the indirect EPR detection of the SEI which plays a crucial role in the performance of lithium batteries and demonstrates the huge potential of EPRoC characterization of new battery materials and device concepts.

Klaus Lips - Helmholtz-Zentrum Berlin
Hahn-Meitner-Platz 1 Berlin, Berlin, 14109 Germany, Email: lips@helmholtz-berlin.de

Probing Local Interactions in Biological Redox Proteins with HYSCORE Spectroscopy: From Semiquinone Studies to Photosynthetic Proteins

Patryk Kuleta[12], Rafal Pietras[1], Anna Wójcik-Augustyn[1], Artur Osyczka[1], and Alizée Malnoë[2]

Department of Molecular Biophysics, Faculty of Biochemistry, Biophysics and Biotechnology, Jagiellonian University, Kraków, PolandDepartment of Biology, Indiana University, Bloomington, IN, USA

Electron transfer reactions in biological redox proteins often involve transient semiquinone (SQ) intermediates whose stability is governed by the local hydrogen-bonding network. Among pulsed EPR techniques, hyperfine sublevel correlation (HYSCORE) spectroscopy is particularly well suited for resolving weak hyperfine interactions that provide direct insight into the local electronic and structural environment of protein-bound radicals.
As an example of this approach, the semiquinone at the quinone reduction (Q_i) site of cytochrome bc_1 was investigated using X-band HYSCORE spectroscopy in combination with quantum mechanical (QM) calculations. A comparison of the wild-type enzyme with the H217R mutant, in which the replacement of a histidine ligand by arginine markedly enhances SQ stability, revealed distinct ^{14}N HYSCORE fingerprints associated with histidine- and arginine-mediated hydrogen bonding. Analysis of ^{14}N hyperfine and quadrupolar interactions, together with ^{1}H hyperfine couplings, enabled assignment of the hydrogen-bond donors surrounding the SQ. The experimentally determined magnetic parameters showed excellent agreement with QM calculations, providing a consistent structural model of the hydrogen-bonding network. Furthermore, the characteristic X-band HYSCORE pattern observed for the H217R mutant identifies spectroscopic features that may serve as diagnostic markers of arginine coordination to semiquinones in other redox proteins.
Beyond elucidating the molecular basis of semiquinone stabilization in cytochrome bc_1, these studies demonstrate the broader potential of HYSCORE spectroscopy for probing structural interactions that govern biological electron transfer. This methodological framework provides a basis for extending pulsed EPR approaches to photosynthetic proteins, including ongoing studies of light-harvesting complex II (LHCII) under high-light and oxidative stress conditions.

Patryk Kuleta - Indiana University
1310, S Woodlawn Ave Bloomington, Indiana, 47401 United States, Email: pkuleta@iu.edu

Dual EPR spin probe and label approach resolves origins of protein and coupled solvent dynamics and confinement-induced folding in fibrillar amyloid-ß(1-42)

Hana Alsheikh,[1] Katie L. Whitcomb,[1] and Kurt Warncke.[1]

Emory University, Department of Physics, Atlanta, GA 30322-2430

Monomeric amyloid-ß (Aß) is an intrinsically disordered protein (IDP), with common lengths of 38-42 residues. Aß forms fibrils with characteristic amyloid cross-ß sheet structure and a disordered N-terminal region (residues 1-17).[1] To gain insight into molecular mechanisms of Aß function and dysfunction in Alzheimer's disease, a dual spin probe and spin label electron paramagnetic resonance (EPR) spectroscopy approach is applied in a frozen solution system,[2,3] that features temperature (*T*) -controlled, ice-boundary confinement. Protein and coupled solvent dynamical properties of Aß42 fibrils are addressed by using the spin-probe, TEMPOL, colocalized with the protein. Spin-labelling with Cu^{2+} at native His6, 13, 14 is used to assess the N-terminal domain dynamics.[4,5] Temperature-dependence (220-265 K) of TEMPOL rotational mobility resolves two correlation times, denoted "fast" (dynamically disordered region) and "slow" (hydration region), with normalized weights, W_f and W_s. The overall decrease in W_f with increasing confinement proceeds in three stages: compaction 1 (C1) - structure consolidation (SC) - compaction 2 (C2). This behaviour is also characterized in fibrils and oligomers of the IDP, a-synuclein.[6] From the Cu^{2+} label perspective, the arrest of Cu^{2+} mobility with decreasing *T* indicates N-terminal domain collapse as the primary C1 origin. Cu^{2+} binding maintains the TEMPOL-detected three-stage compaction but increases C1 extent and shifts SC to lower *T*. These results are consistent with bound Cu^{2+} promotion of N-terminal region disorder. A thermodynamic treatment of the three-stage compaction mechanism provides an approach to quantitative assessment of Aß42–drug interactions. Supported by NIH R01 GM142113.

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Hana Alsheikh - Emory University
400 Dowman Dr Atlanta, Georgia, 30322 United States, Email: halshei@emory.edu

Frequency-Agile Pulse Slicing for High-Field, High-Power, Pulsed Electron Spin Resonance

Alex Giovannone, Casey Bernd, Nick Agladze, Juan Gaitan, Antonin Sojka, Qile Wu, Brad Price, Wei-Hsu (Wish) Lin, Johanna Schubert, Mark Sherwin

The Institute for Terahertz Science and Technology, the University of California - Santa Barbara

A central challenge in realizing pulsed Electron Spin Resonance (ESR) above 100 GHz is generating pulses with sufficient power. At UCSB, we are nearing completion on a unique pulsed ESR spectrometer designed to slice the output of a free-electron laser (FEL) into high-power microwave pulses with independently controllable duration, phase, and amplitude. The FEL can generate kW power for a few microseconds, or 10s of kW in 40 ns pulses when cavity-dumped. We aim to use this source to measure nanosecond lifetimes in the high field regime.

In this talk, I will report on progress in the pulse slicing subsystem of the FEL-powered agile electron spin resonance spectrometer (FELAESR). Pulse slicing is achieved using laser-driven silicon semiconductor switches (LDSS), in which ultrapure silicon wafers with passivated surfaces are driven from a transmissive to a highly reflective state by 532 nm laser pulses. Three broadband stacked complementary-channel pulse slicers, separated by two frequency-agile phase shifters, enable slicing the FEL output into up to three kilowatt-level microwave pulses. I will describe measurements of the insertion loss, leakage between channels, and pulse slicing demonstrations. We measured the pulse slicing system with LDSS whose thickness is designed for optimal performance at 205 GHz and 410 GHz. The frequency-agile phase shifters, which control the relative phase of sub-THz pulses by mechanically varying the path length of one channel, will also be characterized. Together, these subsystems bring our new spectrometer close to its first pulsed ESR measurements on systems with nanosecond relaxation times. This work is supported by NSF DMR 2117994.

Alex Giovannone - University of California - Santa Barbara
Department of Physics - Broida Hall, University of California Santa Barbara, Ca, 93106-9530 United States, Email: alexgiovannone@ucsb.edu

First Experience with Large Volume Resonators for EPR Oxygen Imaging

Daniel J. SantaLucia[1], Boris Epel[1,2], and Mrignayani Kotecha[1]

[1] Oxygen Measurement Core, O2M Technologies, LLC, 2201 W Campbell Park Dr., Chicago, IL 60612, USA
[2]Department of Radiation and Cellular Oncology, The University of Chicago, Chicago, IL 60637, USA

In recent years, electron paramagnetic resonance (EPR) oxygen imaging (EPROI) has demonstrated immense potential in many preclinical biomedical applications. Currently, EPROI technology is limited to mouse and rabbit limb-sized samples, with typical resonator diameters of 1.26”-2.25”, respectively.[1,2] The transition to human scale instead requires resonators 4’’-10” in diameter, with imaging depths reaching 5” or more. To our knowledge, there are no reports of *in vivo* use of such resonators. In this project, we made the first attempt to expand into large-sample EPR imaging. We developed several loop-gap resonators with increasing diameters (the largest of which is 8” in diameter and 4” in length) and demonstrated their performance using deoxygenated crystalline lithium phthalocyanine (LiPc) phantoms as well as with deoxygenated 5 mM and 10 mM trityl OXO71 phantoms. We investigated the impact of using 8, 16, and 24 gaps for 8” resonators, finding little difference in resultant image quality. All experiments used our 9-mT/250-MHz/60-cm bore human-size EPROI instrument, CAELI-9.[2] We obtained preliminary images with ~2 mm spatial resolution using the Ø8”x4” 16-gap resonator. Future work will focus on making large-object EPR imaging practical using lossy samples and smaller practical concentrations of the trityl OXO71 probe.

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Daniel J Santa - O2M Technologies, LLC
2201 W Campbell Park Dr. Chicago, IL, 60612 United States, Email: daniel.santalucia@oxygenimaging.com

Molecular Hyperfine Qubits Based on Heavy Elements

Stephen Hill,[1,2] J. Hruby,[1] D. X. Ngo,[3] P. W. Smith,[4] K. Kundu,[1] K. R. McClain,[5] H. Kwon,[3] Y. J. Franzke,[6] C. A. Gould,[3] B. G. Harvey,[5] S. Minasian,[4] W. J. Evans,[7] J. R. Long[3,4]

NHMFL, Florida State University, Tallahassee, FL 32310, USA Dept. of Physics and Chemistry & Biochemistry, Florida State University, Tallahassee, FL 32306, USA Depts. of Chemical & Biomolecular Engineering, UC Berkeley, CA 94720, USA Materials Division, LBNL, Berkeley, CA 94720, USAUS Navy, Naval Air Warfare Center, China Lake, CA 93555, USA Fachbereich Chemie, Philipps-Universität Marburg, 35032 Marburg, GermanyDepartment of Chemistry, UC Irvine, Irvine, CA 92697, USA

Recent work on molecular spin qubits has demonstrated significant enhancements in coherence through the engineering of so-called clock transitions, optimal operating points at avoided Zeeman level crossings where the quantum spin dynamics become desensitized to magnetic noise [1]. The first examples focused on clock transitions generated by off-diagonal terms in the crystal-field Hamiltonian of integer spin-orbital (*J*) moment lanthanide (Ln) ions (primarily Ho^{III}) in axial coordination environments – integer because the off-diagonal terms are even in angular momentum operators, therefore lifting the degeneracies within quasi-doublet, $m_J = \pm i$, projection states (i = integer). Unfortunately, the optimum coherence times (T_2) observed in such systems are severely limited by spin-lattice (T_1) relaxation due to the strong spin-orbit coupling (SOC) present in open-shell f-elements. This has motivated investigations of heavy elements with half-integer moments, where the clock transitions are generated instead via the off-diagonal part of the hyperfine interaction. In the case of lanthanides, a key trick involves reduction to the 2+ oxidation state which, for lutetium, results in a $4f^{14}(5d/6s)^1$ electronic configuration, i.e., a filled f-shell, with the extra electron occupying a mixed 5d/6s orbital, giving rise to a relativistically enhanced contact hyperfine interaction due to the s-orbital occupancy. Moreover, by increasing the overall s-orbital character, one can reduce SOC and enhance T_1 [2]. After an introduction, this talk will review recent work focusing on a general class of compounds that can be viewed as "*molecularly trapped ions*", in analogy to the trapped species currently employed in some of the most advanced quantum computing devices. Examples include recent efforts targeting enhanced s-orbital character in linear bis-cyclopentadienyl Lu^{II} complexes [3], as well as other Ln^{II} complexes with $4f^n(5d/6s)^1$ electronic configurations [4]. Time allowing, more exotic examples will be discussed.

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Stephen Hill - Florida State University and NHMFL
77 Chieftan Way Tallahassee, FL, 32306 United States, Email: shill@magnet.fsu.edu

Elucidating Electronic Structure and Relaxation Pathways of Transition Metal Qubits via High Power EPR Spectroscopy

Kavipriya Thangavel,[1] Dipanti Borah,[2] Vignesh Kasi,[2] Maheswaran Shanmugam,[2] Andreas Pöppl[3], Stephen Hill[1,4,5]

National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USADepartment of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076, IndiaFelix Bloch Institute of Solid State Physics, University of Leipzig, 04103 Leipzig, GermanyDepartment of Physics, Florida State University, Tallahassee, FL 32306, USADepartment of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306, USA

Molecular spin qubits, known for their precise control, scalability, tunability, and room-temperature capability to sustain multiple quantum states, are promising candidates for quantum information science [1]. These systems enable large-scale production, precise tuning of spin environments, and arrangement into 2D or 3D lattices. Progress in their design and integration is crucial for overcoming challenges related to addressability, coherence, and scalability in future quantum technologies. In this context, metal–organic frameworks (MOFs) have recently gained attention as tunable platforms for molecular qubits. Among them, the breathing MOF MIL-53 [2] has emerged as a promising material for quantum information science applications [3].
In this context, we performed high-field continuous-wave (CW) electron paramagnetic resonance (EPR) experiments up to 413 GHz on Co(II)-based metal complexes and a Cr(III)-based MOF to probe their electronic and structural properties. Two low-spin Co(II) (S = 1/2) complexes, [CoCl(DPPE)2]SnCl3, with square pyramidal (Co-SP) and trigonal bipyramidal (Co-TBP) geometries, exhibited distinct EPR signatures arising from their different coordination environments. High-power W-band EPR (HiPER) measurements further revealed temperature-dependent relaxation behavior up to 60 K. At 5 K, Co-TBP showed $T2$ ˜ 5.8 µs and $T1$ ˜ 0.62 ms, while Co-SP exhibited $T2$ ˜ 3.5 µs and $T1$ ˜ 0.98 ms. For MIL-53, $T2$ and $T1$ were approximately 0.96 µs and 50 µs, respectively, at 5 K. Furthermore, field-dependent relaxation measurements covering the S = 3/2 spectral features, together with field-dependent ELDOR-detected nuclear magnetic resonance (EDNMR) experiments, were performed to elucidate the relaxation behavior of different transitions and probe the surrounding nuclear spins, respectively.

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Kavipriya Thangavel - National high Magnetic Field Laboratory
1800 E Paul Dirac Dr, Tallahassee, Florida, 32310 United States, Email: kt24@fsu.edu

Multi-Mode Spin-Rabi Oscillation of Strongly EPR Driven Electron Spins Pairs in the Landau Zener Regime

B. A. Odeke,[1] P. Poudel,[1] A. Ahmad,[1] C. Pak,[1] C. Dhakal,[1] D. Mansfield,[2] R. Stolley,[2] C. Boehme.[1]

1. Department of Physics &; Astronomy, University of Utah, 270 S, 1400 E, Salt Lake City, UT 84112, USA
2. Department of Chemistry, University of Utah, 315 S,1400 E, Salt Lake City, UT 84112, USA

Electron spin-Rabi oscillations due to electron paramagnetic-resonant (EPR) driven by a linearly polarized, radio-frequency domain oscillating magnetic field with amplitude B_1 in excess of both, a static magnetic Zeeman field B_0 and local random hyperfine fields, have been predicted to give rise to long-lived charge carrier spin pair states.[1] To test this experimentally, we performed strong-drive pulsed electrically detected magnetic (EDMR) resonance experiments at room temperature and low B_0 < 0.5mT. To observe EPR via electric current, we used spin-dependent polaron recombination currents in bipolar injection devices, essentially organic light emitting diodes (OLEDs), based on the perdeuterated p-conjugated polymer *poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene]* MEHPPV. Our experiments revealed that the Rabi nutation transient exhibited higher harmonics caused by drive passage induced Landau-Zener transitions, whose number *N* increases linearly with *B*1, following the relation |4*B*1/*B*0|, as predicted by theory. Also, as predicted by theory, the observed oscillatory behavior continues on the time scale of milliseconds, indicating strong coherence protection due to the emergence of spin-Floquet states.[2]

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Bonaventure Odeke - University of Utah
270 S, 1400 E Salt Lake City, Utah, 84112 United States, Email: bonaventure.odeke@utah.edu

Confining Molecular Spin Qubits in Two-Dimensional Solid-State Architectures

Anna Champ,[1] Eleanor Mackintosh,[1] André Koch Liston,[1] Sanghyo Lee,[2] Eric D. Walter,[3] Raphaël P. Hermann,[4] Augustin Braun,[1] Willa Mihalyi-Koch,[1] Jeffrey M. McNeill,[1] Daniel G. Chica,[1] Johan van Tol,[5] Tomas Orlando,[5] Mykhaylo Ozerov,[5] Byeongjun Gil,[2] Myung-Geun Han,[2] Jonathan S. Owen,[1] Timothy C. Berkelbach,[1] Milan Delor,[1] Michael L. Steigerwald,[1] Colin Nuckolls,[1] Xavier Roy,[1] Arun Ramanathan[1]

1. Columbia University, Department of Chemistry, New York, NY 10027, USA
2. Brookhaven National Laboratory, Condensed Matter Physics &; Materials Science, Upton, NY 11973, USA
3. Pacific Northwest National Laboratory, Environmental Molecular Sciences Laboratory, Richland, Washington 99352, USA
4. Oak Ridge National Laboratory, Materials Science and Technology Division, Oak Ridge, TN 37831, USA
5. National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA

Molecular spin qubits (MSQs) offer a chemically tunable platform for quantum sensing and information processing, yet their integration into solid-state environments remains limited by rapid decoherence induced by surface interactions and environmental noise.[1] Here, we introduce van der Waals (vdW) confinement within layered two-dimensional materials as a general strategy to stabilize and enhance coherence in MSQs. Using reductive intercalation, we confine cobaltocene ($CoCp_2$) molecules within the vdW gaps of diamagnetic semiconductors SnS_2 and $CdPS_3$, forming self-assembled mixed-valence superlattices in which a subset of $^{59}Co^{2+}$ centers act as addressable S = 1/2 qubits. Comprehensive structural and spectroscopic characterization confirms successful confinement, charge transfer, and preservation of the host lattice framework. Continuous-wave electron paramagnetic resonance (EPR) measurements show that confinement dramatically alters the electronic structure of CoCp2, indicating substantial reorganization of its local electronic environment within the vdW gap. Probing the spin dynamics with pulsed EPR methods, we observe an increase in spin-lattice relaxation time (T_1) by three orders of magnitude compared to molecular crystals, along with measurable signals up to 100 K. The phase memory (T_m) of vdW confined molecules shows similar substantial enhancement, but only a weak temperature dependence as it traces T_1 with measurable echo up to 100 K, above which T_m is limited by T_1. We attribute the enhanced coherence upon confinement to the increased Jahn-Teller distortion due to non-covalent interactions between the host and the guest. These results establish vdW confinement as a powerful design strategy for engineering spin coherence in molecular systems, providing a pathway toward atomically precise, scalable quantum sensing hybrid architectures with deterministic placement and controlled orientation of MSQs.

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Anna Champ - Columbia University
3000 Broadway New York, New York, 10027 United States, Email: aec2262@columbia.edu

Photoexcited transient EPR of tetrakis(4-carboxyphenyl)porphyrin (TCPP), with differing ions, as ligands in zirconium MOFs towards quantum sensors and DNP transfer

Wern Ng[1], Jacob M. Lessard[2], Prathami Divakar Kamath[3], Chongwei Zhang[1], Jessica Yujie Wu[1], Ah-Young Song[1], Emanuel Druga[1], Kyriakos C. Stylianou[2], Jeffrey A. Reimer[1], Ashok Ajoy[1]

1. Department of Chemistry, University of California, Berkeley, CA, USA
2. Materials Discovery Laboratory (MaD Lab), Department of Chemistry, Oregon State University, Corvallis, OR, USA
3. Department of Materials Science and Engineering, University of California, Berkeley, CA, USA

Molecules with strong electron spin polarization have been used as quantum sensors and for enhancing nuclear spins through dynamic nuclear polarization (DNP)[1,2]. However, despite strides in transferring such polarization to more common chemical systems, the overall enhancement factors can still be improved. We here analyze the triplet electron spin dynamics of tetrakis(4-carboxyphenyl) porphyrin (TCPP) linkers within the zirconium based MOF-525 at room temperature and cryogenic temperatures using a homebuilt electron paramagnetic resonance (EPR) spectrometer at X-band. The transient EPR signals are detected from the porphyrin triplet states after pulsed laser excitation at 527 nm. We will present the effects of differing metal ions within the porphyrin linkers on the electron spin lattice relaxation times, alongside population analysis of the triplet sublevels. The incorporation of the triplet molecule as a linker within the MOF, coupled with the biocompatibility of MOF-porphyrins[3], strives towards realizing “bulk-as-sensing” platforms that may utilize DNP on adsorbed analytes for sensing. Longer relaxation times would be advantageous for bestowing the electron spin polarization to analytes adsorbed onto the MOF.
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Wern Ng - University of California Berkeley
University of California Berkeley, Tan Kah Kee Hall Berkeley, California, 94720 United States, Email: wern.ng@berkeley.edu

Magnetic resonance studies of poly-rotaxanes based on inorganic rings

Eric J. L. McInnes

The University of Manchester

Supramolecular chemistry has produced remarkable structures and functional molecules, as recognised by the award of the 2016 Nobel Prize for Chemistry to the pioneers of molecular machines. Most of this chemistry has been based on organic chemistry, for example, the rotaxanes based on long-chain molecules threading through macrocycles. We have been studying supramolecular structures where the molecular components are themselves complex inorganic molecules containing many paramagnetic transition metal ions.[1] Such molecules have attracted interest due to their unusual physics. In this talk I will describe systems based on molecules of general formula $(R_2NH_2)[M^{III}_7M'^{II}F_8(O_2CR')_{16}]$. These complexes can be extended to supramolecular structures, for example using the M_7M' ring as the macrocyclic component of rotaxanes. Following such approaches huge structures containing hundreds of paramagnetic metal ions can be prepared. EPR and NMR techniques (and complementary methods) are used to explore the intra- and supra-molecular interactions which range from THz to MHz scales, and their solution chemistry.

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Eric McInnes - The University of Manchester
Oxford Road Manchester, Greater Manchester, M13 9PL United Kingdom, Email: eric.mcinnes@manchester.ac.uk

LLM-Assisted Modular Instrumentation: ODNP as a Case Study

John M. Franck[1], Atahan Garip[2]

ACERT, Ithaca, NY 14850Cornell University, Applied Engineering and Physics, Cornell, NY 14850

The implementation of new types of magnetic resonance spectroscopy frequently requires the synchronization and programming of several independent instrumental modules. Researchers have historically reached for graphical control stacks such as LabVIEW as an efficient work-around to the high barrier of entry of written programming languages. Large language models (LLMs) invert that calculus: with strategic guidance, an LLM constructs a fully-fledged control module for a new piece of instrumentation in a few hours, given the device's programming manual along with a specified set of requirements about the code to be written. More importantly, freedom from the tedium of manually translating manuals into working code opens access to higher-level programming concepts such as class inheritance, context managers, TCP/IP inter-process communication, operator overloading, and unit-test suites — each illustrated here with concrete examples[1]. An integrated, code-first control architecture built on this approach synchronizes, in a single Python codebase, NMR pulse-program execution, high-power microwave control, static-field manipulation, continuous logging of forward and reflected microwave power, and real-time feedback adjustment. To provide concrete examples, we use our codebase for running automated ODNP experiments. These include measurements of the ODNP enhancement and the ODNP-detected T_1 as a function of microwave power, as well as field-domain EPR spectra recorded via ODNP enhancement. The low barrier to advanced coding strategies enables such experiments on a reused room-temperature electromagnet that an off-the-shelf current source drives directly through software[2]. The talk concludes by integrating these developments with our recently published general theory for predicting signal and noise power in unconventional NMR setups[3] — a theory rooted in the long history of EPR instrumentation theory — and outlines how the resulting platform anchors our next-generation ODNP/EPR spectrometer. This code-first, LLM-assisted approach lowers the barrier to multi-modal EPR/DNP instrumentation community-wide.

Atahan Garip - Advanced Center for ESR Research and Technology
206A Dryden Rd #107 Ithaca, NY, 14850 United States, Email: ag2639@cornell.edu

EPR Characterization of Redox- and Topology-Dependent Spin Coupling in Diboron-Incorporated Indenofluorenes

Yujie Zhao, Bi Youan E Tra, Colleen H. McAloon, Andrew Molino, Chunlin Deng, Yifu Ouyang, Peter Mullër, David Wilson, Robert Griffin, Robert Gilliard

Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139, USA

Boron-doped polycyclic p-systems provide a flexible platform for tuning open-shell electronic structure, but assigning the spin state requires direct magnetic resonance characterization. Here, continuous-wave and pulsed EPR spectroscopy are used to examine spin coupling and spin delocalization in diboron-incorporated indenofluorene radicals and diradicals. In ligand-stabilized diboraindeno[1,2-b]fluorenes, chemical reduction gives open-shell singlet diradicals with thermally accessible triplet states. X-band CW EPR and Q-band echo-detected field-sweep measurements show triplet features together with an S = 1/2 monoradical impurity contribution. Microwave power-dependent CW EPR and nutation experiments were used to resolve the triplet signal and support the S = 1 assignment. In a second family of aryl-substituted diboron indenofluorene isomers, removing strongly p-accepting carbene ligands shifts the electronic structure toward the conjugated molecular core. The EPR-active meta-quinodimethane-like DB[2,1-b]IF reduced species include a 19p radical anion and 20p triplet diradicals. The radical anion shows boron and proton hyperfine couplings consistent with spin delocalization across the p-framework, while the triplet diradicals display small zero-field splitting parameters, indicating weak dipolar coupling between delocalized spins. In contrast, the para-quinodimethane-like DB[1,2-b]IF dianion favors a closed-shell singlet structure and serves as a useful comparison. Together, these studies show how EPR distinguishes radical impurities, doublet radicals, triplet diradicals, singlet–triplet energetics, and ligand-versus-core spin delocalization in main-group open-shell molecules.

Yujie Zhao - Massachusetts Institute of Technology
170 Albany Street, NW14 Francis Bitter Laboratory Boston, MA, 02139 United States, Email: yujiez@mit.edu

Electrically detected ferromagnetic resonance evidence for orbital angular momentum transport in an organic semiconductor

P. Poudel[1], P. Bailey[1], P. Bissokarma[1], J.S. Miller[2], E. A. Montoya[1], Z.V. Vardeny[1], and C. Boehme[1]

[1] Department of Physics and Astronomy, University of Utah, Salt Lake City, Utah 84112, USA and
[2] Department of Chemistry, University of Utah, Salt Lake City, Utah 84112, USA

Pure spin-current injection driven by ferromagnetic resonance (FMR) has become an important spectroscopic approach for studying angular momentum transport in condensed-matter systems, including organic semiconductors[1]. In these experiments, microwave excitation of a ferromagnetic injector generates nonequilibrium spin or angular momentum currents that are detected electrically through Hall-type conversion processes in adjacent detector layers. Organic semiconductors have attracted particular interest because weak spin–orbit coupling can lead to long spin-relaxation times, although the strongly localized nature of charge transport in molecular solids raises important questions regarding the microscopic origin of the transported magnetization[2]. Recent studies have demonstrated that orbital angular momentum can also be generated and detected in FMR-based experiments through orbital pumping and orbital Hall conversion mechanisms[3,4]. Here, we present electrically detected ferromagnetic resonance experiments on multilayer structures containing the prototypical organic semiconductor tris(8-hydroxyquinolinato) aluminium (Alq_3) combined with injector and detector materials selected for their differing sensitivities towards spin and orbital angular momentum. By systematically comparing injector–detector combinations, angular dependencies, and spacer-free control structures, we isolate the contribution arising from magnetization transport through the organic layer. The resulting hierarchy of electrically detected Hall-type signals is found to be inconsistent with predominantly spin-mediated transport and instead indicates that orbital angular momentum constitutes the dominant transported quantity in Alq3. These results demonstrate how magnetic-resonance techniques can distinguish spin and orbital contributions to angular momentum transport in molecular materials.

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Prashanna Poudel - University of Utah
275S University St. W2224 Salt Lake City, UT, 84092 United States, Email: u0510101@physics.utah.edu

Sub-Terahertz Characterization of Anodic Aluminum Oxide Wafers for use in Liquid Sample High-Field EPR Resonators

Johanna Schubert[1], Nick Agladze[1], and Mark Sherwin[1]

1. University of California at Santa Barbara, Santa Barbara, CA, 93106.

(Sub-)Terahertz high-field electron paramagnetic resonance (EPR) spectroscopy of aqueous samples is severely limited by high dielectric losses associated with the high-frequency edge of the water Debye relaxation peak. Recently, the Sherwin Lab has used resonator-free quasioptics for measuring time-resolved inter-residue distance changes in proteins at high fields (8.6 T, 240 GHz), mitigating loss by utilizing thin sample geometries such as a 100 micron thickness protein solution held within Vitrocom rectangular borosilicate glass capillaries [1]. Implementing a cost-effective resonator into a quasi-optical sample holder that minimizes parasitic cross-polar signals remains a significant challenge [2]. Here, I evaluate using anodic aluminum oxide (AAO) wafers in a planar, asymmetric Fabry-Perot geometry. AAO is believed to mitigate dielectric loss of water in the (sub-)THz range [3] and can be PEGylated to achieve biocompatibility. InRedox AAO wafers (~15% porosity) of various pore diameters (20, 40, 80, 120, 160 nm) were characterized via vector network analyzer transmission measurements from 220 to 310 GHz. 3D-printed PLA clamps and thin (~22 micron) polypropylene sheets were used to mount wafers and measure single and stacked transmission across ambient moisture and water-filled treatments, the latter relying on the Marangoni effect with isopropyl alcohol and deionized water baths. The transfer matrix method was used to determine effective refractive indices of the wafers, and a naive simulation of two water-filled AAO wafers separated by approximately a quarter wavelength at 240 GHz predicted a Fabry-Perot cavity with a loaded Q-factor of ~ 10. With optimal filling factor, this could yield a 100-fold enhancement in time resolution. While preliminary work shows AAO can act simultaneously as loss-mitigating sample substrate and resonator boundary, current work focuses on modeling the spatial distributions of electric and magnetic field profiles at resonator interfaces, with the goal of integrating AAO in a resonator design that maximizes the magnetic field and minimizes the electric field at the sample location.

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Johanna Schubert - University of California, Santa Barbara
1311 Broida Hall Santa Barbara, California, 93106 United States, Email: johannaschubert@ucsb.edu

Structural and Functional Characterization of the Diiron Protein ScdA from *Staphylococcus aureus*

Yun-Wei Chiang

National Tsing Hua University, Department of Chemistry, Hsinchu 300-044, Taiwan

Staphylococcus aureus ScdA has been traditionally implicated in protecting bacterial cells against oxidative and nitrosative stress through the preservation of iron–sulfur cluster integrity. In this study, we employ an integrative structural biology approach combining X-ray crystallography, NMR spectroscopy, electron spin resonance (ESR), and AlphaFold-based modeling to determine the full-length structure of ScdA and to uncover an unexpected enzymatic function.[1] Our structural analyses reveal that ScdA forms a homodimeric assembly stabilized by a flexible linker domain that mediates extensive hydrophobic contacts and hydrogen-bonding interactions between subunits. Remarkably, biochemical assays together with EPR measurements demonstrate that ScdA is capable of catalyzing the reduction of nitrite to nitric oxide (NO) in vitro. Consistent with this activity, heterologous overexpression of ScdA in Escherichia coli leads to pronounced growth inhibition under nitrite stress conditions in vivo. These findings challenge the prevailing view of ScdA solely as a defensive factor against nitrosative stress and instead suggest a multifunctional role in which a single di-iron center supports both iron–sulfur cluster maintenance and NO generation. Elucidating the regulatory mechanisms and physiological contexts that govern this functional duality will be essential for understanding ScdA activity in S. aureus.[2] Collectively, our results establish ScdA as a versatile di-iron protein and highlight its potential as a target for the development of novel antimicrobial strategies.

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Yun-Wei Chiang - National Tsing Hua University
101, Sec 2, Kuang-Fu RD Hsinchu, Hsinchu, 300044 Taiwan, Email: ywchiang@mx.nthu.edu.tw

EPR with Imaging for batteries

Bingwen Hu,[1] Fushan Geng,[1] Xiaobing Lou[1]

1. East China Normal University, Department of Physics, Shanghai, 200433 China

We utilize EPR and EPR imaging to investigate the structure-performance relationship of rechargeable batteries.
(1) In Situ EPR Imaging
We have developed in situ EPR imaging, which enables the top-view observation of lithium deposition.[1] We investigated lithium dendrite growth on graphite and found that overcharging leads to the formation of long dendrites prone to separator penetration.[2] We also use EPR imaging for Li-metal anode.[3] For all-solid-state batteries, we established in situ L-band EPR imaging and discovered that ring-shaped lithium foil anodes exhibit significantly superior performance compared to conventional circular lithium foil anodes.[4] Furthermore, using 3D EPR imaging for the first time, we revealed that composite solid electrolytes can suppress lithium dendrite penetration through the electrolyte.[5] We also employed EPR to study sodium deposition on KJB carbon-coated copper foil and the effect of the separator with two layers on Na plating.[6,7]
(2) Molecular O2 Detection by EPR
The prevalent resonant inelastic X-ray scattering (RIXS) method may fail to distinguish between molecular O2 and Ru–O2(d?) species. However, EPR has been validated to detect trapped molecular oxygen in the cathode Li2Ru?Sn1??O3 and differentiate between these two states.[8] Moreover, in the fully strongly coupled system Li2RuO3, we found that strong magnetic frustration drives the formation of molecular O2 and O2n?.[9] This mechanism of magnetic frustration promoting molecular oxygen generation was also verified in Li1.2Ni0.2Mn0.6O2, and found to be correlated with Ni/Mn cation mixing.[10] At last, EPR and magnetic frustration were used for high Ni system $LiNi_xMn_{1-x}O_2$, showing that the maximum Ni content is 91.6% with better thermal stability.[11]

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Bingwen Hu - East China Normal University
Dongchuan Road 500, Optics Building, B519 Shanghai, Shanghai, 200433 China, Email: bwhu@phy.ecnu.edu.cn

From diamond defects to protein-based qubit sensors

Peter Maurer

The University of Chicago

Quantum metrology enables some of the world's most sensitive measurements with potentially far-reaching applications in the life sciences. Although the ultrahigh sensitivity of qubit sensors has sparked the imagination of researchers, implementing them in actual devices that enable monitoring cellular processes or detecting diseases remains largely elusive. Overcoming the limitations that hinder the broader application of quantum technology in the life sciences requires advances in both fundamental science and engineering. In this talk, I will discuss new strategies that combine quantum engineering and molecular biology to develop a new generation of quantum sensors that can be readily integrated with biological systems. My discussion will start with the development of a novel biocompatible surface functionalization architecture for highly coherent diamond crystals. I will then continue with discussing a new approach to engineering spin coherence in core-shell structured diamond particles, which can be readily chemically modified and delivered to intact biological systems. Finally, I will depart from established diamond sensors and introduce an entirely new class of biological qubits based on optically-addressable spins in fluorescent proteins. These protein-qubits have coherence times and optical readout comparable to solid-state defects, but are only 3 nm in diameter and genetically encodable. The unifying theme of these advances is the convergence of techniques from quantum engineering and molecular biology. Specific applications of the developed sensing platforms to questions in the life sciences will be discussed throughout this talk.

Peter Maurer - The University of Chicago
5801 S Ellis Avenue Chicago, IL, 60637 United States, Email: pmaurer@uchicago.edu

Rotor-synchronized Magic Angle Spinning EPR Experiments at 7 and 14 Tesla

Ilia Kaminker

School of Chemistry, Tel-Aviv University, Tel-Aviv, Israel

High-field EPR is essential for an in-depth understanding of Dynamic Nuclear Polarization (DNP) – a prominent technique for signal enhancement in contemporary NMR. DNP is based on polarization transfer from an unpaired electron spin to neighboring nuclear spins. Since DNP performance depends on experimental conditions, typical low-field static EPR experiments are of limited relevance for studying modern, high-field Magic Angle Spinning (MAS) DNP, which requires the development of high-field pulsed MAS-EPR instrumentation and methodology. Recently, we reported the first high-field (7 T) pulsed MAS-EPR experiments at spinning rates up to 3 kHz[1]. In this work, we demonstrate MAS EPR experiments at spinning speeds up to 37 kHz and magnetic fields up to 14 T. In particular, the development of rotor-synchronized stimulated-echo MAS-EPR experiments allows for observation of electron spin dynamics on the hundreds-of-microsecond timescale. This expands the timescale available for the MAS-EPR investigation of DNP mechanisms by two orders of magnitude compared to a simple two-pulse echo experiment. This allows us to observe polarization exchange between different electron spins, an essential process predictive of DNP efficiency. Beyond investigating the DNP mechanism, we demonstrate the unique capability of MAS-EPR to separate EPR spectra by anisotropy.

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Ilia Kaminker - Tel Aviv University
Haim Lebanon 55 Tel Aviv, CEnter, 6997801 Israel, Email: iliakam@tauex.tau.ac.il

High field microfluidic NMR spectroscopy by longitudinal magnetization detection with pulsed NV magnetometry

Janis Smits[1], Bryan Richards[1], Yaser Silani[2], Andrew McDowell[3], Andrey Jarmola[4], Victor Acosta[1]

Center for High Technology Materials, University of New Mexico, Albuquerque, New Mexico, United StatesDepartment of Electrical and Computer Engineering, University of Washington, Seattle, Washington NuevoMR, Albuquerque, NM, USA ODMR Technologies Inc., El Cerrito, CA

The power of NMR spectroscopy as a quantitative analysis tool across multiple disciplines has been well established. Its main drawback is a relatively poor sensitivity when compared to mass-spectrometry, especially in scenarios where the analyte concentrations and volumes are small. This is almost always the case in fields such as metabolomics, which has prompted the development of magnet systems that can produce higher field and microcoils capable of detecting smaller quantities of analyte.
The nitrogen-vacancy (NV) center in diamond can be a strong competitor to NMR microcoils when performing NMR spectroscopy on small volumes (<1nL). The sensor is optically addressed which enables magnetometry at the optical diffraction limit thus being a natural fit for small volume NMR. Here we present some preliminary work showing NV NMR spectra at a moderate field of ~0.5 T using a Ramsey-ENDOR protocol. The magnetometer itself has a photon shot-noise limited magnetic sensitivity of ~5pT?$s^{1/2}$ which equates to a proton molar sensitivity of ~ 12M for an SNR of 3 at a bias field of 0.5 T. These results build on previous published work[1] showing using the Ramsey-M_z protocol, with the key improvement being the more than an order-of-magnitude improvement in magnetic sensitivity achieved by using a Hahn-Echo measurement on the NVs to read out the nuclear magnetization signal.

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Janis Smits - University of New Mexico
1313 Goddard st SE Albuquerque, New Mexico, 87106 United States, Email: smitsjanis@gmail.com

Next-Generation EPR: Combining High-Performance Q Band Instrumentation with Artificial Intelligence Enhanced Spectral Processing

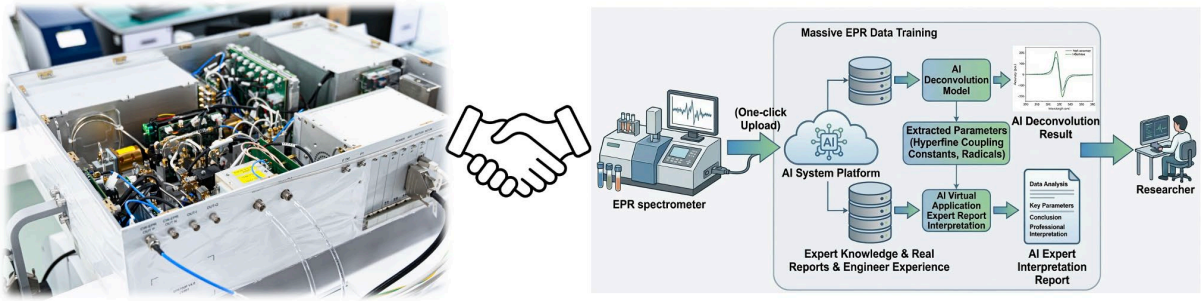
Yang Zhou, Zhuoyang Qin, Yue Zhang, Zhiyu Jeff Sun, Zhifu Richard Shi, Kebiao Xu

CIQTEK Co., Ltd., No. 1969, Kongquetai Road, HeFei High Tech Zone, AnHui, China

The advancement of Electron Paramagnetic Resonance spectroscopy is increasingly defined by the convergence of robust hardware and intelligent software. While EPR remains a vital tool for probing paramagnetic centers, broader adoption is limited by instrument complexity and the steep learning curve of spectral analysis. Researchers at CIQTEK address these barriers by developing high-performance hardware alongside the first dedicated AI model for EPR.

Our Q-band pulsed EPR system achieves less than 10 ns π/2 pulse wide-bandwidth excitation using a Solid-State Power Amplifier, offering superior longevity and reduced maintenance over conventional technology. This architecture maximizes sensitivity and spectral resolution, deciphering complex metal hyperfine couplings and extracting dipolar information for high-resolution DEER distance mapping.
Complementing the hardware is a three-layer AI EPR model that streamlines the workflow from raw data to publication. Trained on over 100,000 real and simulated datasets — achieving 99.9% precision for simulations and 92% for real-world samples — the model automates spectral fitting, component characterization, and experimental report generation. It further offers predictive guidance, suggesting follow-up experiments to validate findings.

This integrated approach lowers the entry barrier for researchers in chemistry, biology, and materials science, driving EPR toward a more impactful technology.



Zhiyu Sun - CIQTEK
No. 1969, Kongquetai Road, High-tech Zone Hefei, Anhui, 230088 China, Email: xiaxy@ciqtek.com

Fourier Transform EPR Spectroscopy Revisited

Dmitry Akhmetzyanov,[1] Timothy Keller,[1] Yen-Chun Huang,[1] Joshua Hoy,[1] and Thorsten Maly[1]

1. Bruker BioSpin Corp., 15 Fortune Drive, Billerica, Massachusetts, 01821, United States

Advancements of pulse shaping techniques in EPR spectroscopy enable novel applications in structural biology, materials science as well as quantum information science.[1] From instrumentation perspective, besides fast arbitrary waveform generators, Q-band loop-gap resonators, serving at the back end of pulse shaping, are crucial as they are capable of achieving bandwidths exceeding 400 MHz, while maintaining high conversion factor and B_1 homogeneity. Furthermore, they benefit from high sensitivity at Q-band frequencies (34 GHz). These developments are important milestones, as spectra of most organic radicals, materials defects and metals in specific cases well match the bandwidth that provides leaps in sensitivity, resolution and experimental capabilities. As such, EPR is positioned amongst tools for advancement of early-stage spin-based quantum technologies, besides its conventional applications.
Engineered materials defects are unique as they introduce quantum systems onto a platform in controllable fashion that allows development of scalable quantum devices (quantum processing units) as well as quantum sensors. Being an integral part of industrial fabrication ecosystem, silicon carbide (SiC) is one of the most promising platforms that can host different types of quantum systems.
In this work we proposed Fourier Transform (FT) EPR-based methods as an efficient tool for studying spin properties in nitrogen doped SiC sample hosting different types of nitrogen systems. We utilized WURST shaped pulses[2] and Q-Band probeheads with large bandwidth for reconstructing EPR spectra with high fidelity as well as for selective and broadband spin inversion. Furthermore, we adopted a domain-colored coherence transfer (DCCT) technique, originally proposed in NMR spectroscopy,[3] that is highly effective for coherence pathway read-out and allows for selection of weak signals.
The FT EPR-based strategies proposed in this work are applicable for wide range of systems and useful for advancement of novel quantum devices enabling efficient characterization of their properties and for other applications in quantum information science.

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Dmitry Akhmetzyanov - Bruker BioSpin Corp.
15 Fortune Drive Billerica, Massachusetts, 01821 United States, Email: dmitry.akhmetzyanov@bruker.com

Expanding Applications of EPR Oximetry with the Ox071 Spin Probe: From Tumor Oxygen Imaging to Detection of Kidney Injury

Shun Kishimoto[1,2], Nallathamby Devasahayam[1], Gadisetti V. R. Chandramouli[3], Murali C. Krishna[1]

[1]Radiation Biology Branch, Center for Cancer Research, NCI, Bethesda, Maryland, USA
[2]Urologic Oncology Branch, Center for Cancer Research, NCI, Bethesda, Maryland, USA
[3]GenEpria Consulting Inc., Columbia, Maryland, USA

Tissue oxygenation plays a critical role in many biological processes, including tumor progression, therapeutic response, and organ injury. However, quantitative and spatially resolved measurement of tissue oxygen partial pressure (pO2) in vivo remains challenging. Electron paramagnetic resonance (EPR) oximetry enables direct mapping of tissue oxygen levels by measuring oxygen-dependent changes in the relaxation rate of paramagnetic spin probes.

Recent advances in trityl radical probes have expanded the capabilities of EPR oxygen imaging. Ox071, a deuterated analog of the widely used Ox063 probe, exhibits improved signal characteristics that allow more reliable measurements of tissue oxygen across both hypoxic and normoxic ranges. Compared with Ox063, Ox071 provides stronger signal intensity and slower signal decay, resulting in improved signal-to-noise ratio and more accurate detection of oxygen distributions in vivo.

Using time-domain EPR imaging with Ox071, we obtained high-resolution three-dimensional oxygen maps in living mice. In tumor models, Ox071 enabled improved characterization of spatial oxygen heterogeneity, revealing oxygenated regions that were difficult to detect with earlier probes. In normal organs such as the kidney, Ox071 imaging clearly resolved the physiological oxygen gradient between the highly oxygenated renal cortex and the relatively hypoxic medulla.

We further applied Ox071-based EPR oximetry to investigate renal oxygenation in a mouse model of chemotherapy-induced acute kidney injury. Longitudinal imaging revealed dynamic changes in kidney oxygenation after cyclophosphamide treatment. These changes correlated with histological evidence of renal damage and showed that urinary pO2 does not reliably reflect tissue oxygenation following tubular injury.

Together, these studies demonstrate that Ox071-based EPR imaging provides a powerful approach for non-invasive, quantitative mapping of tissue oxygenation and may enable new imaging biomarkers for oxygen-dependent diseases and treatment responses.

SHUN KISHIMOTO - NCI
9000 Rockville Pike Bethesda, MD, 20894 United States, Email: shun.kishimoto@nih.gov

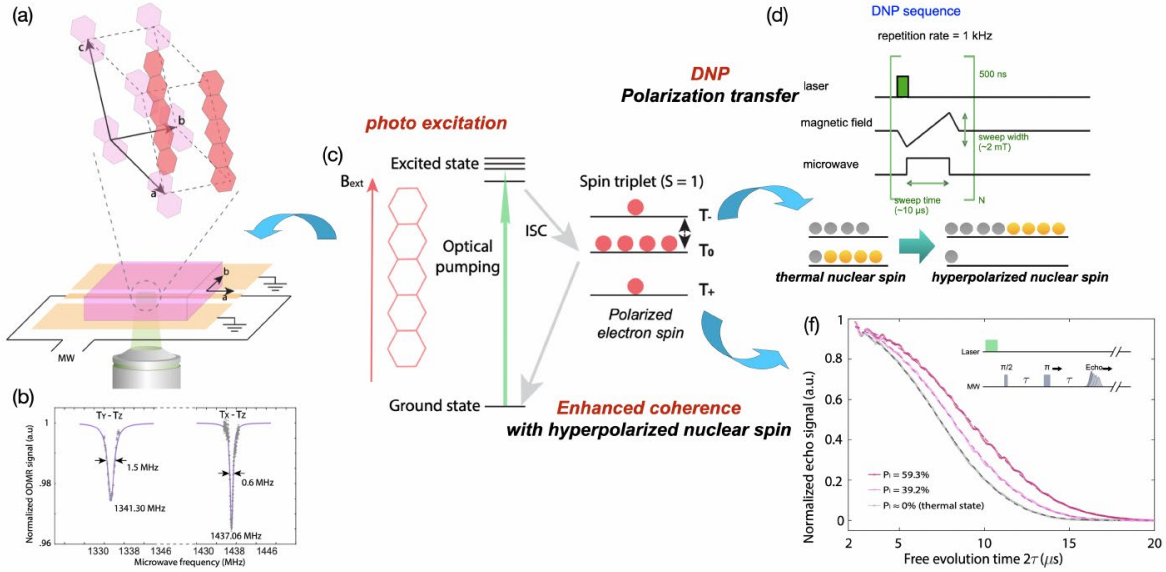
Robust AC Vector Sensing with Pentacene and Enhancing Spin Coherence by Nuclear Spin Hyperpolarization

Boning Li,1 Patrick Hautle,2 Duhan Zhang,3 Tom Wenckebach,2 Paola Cappellaro,1 and Yifan Quan3

1Department of Physics, Massachusetts Institute of Technology, MA 02139, USA
2PSI Center for Neutron and Muon Sciences, CH-5232 Villigen-PSI, Switzerland
3Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA

Molecular spin based quantum sensors offer a range of advantages, from high spin density to functionalization via chemical tunability. Here, we demonstrate microwave vector magnetometry using the photoexcited spin triplet of deuterated pentacene molecules, operating at zero external magnetic field and room temperature. We achieve full three-dimensional microwave field reconstruction by detecting the Rabi frequencies of anisotropic spin-triplet transitions associated with two crystallographic orientations of pentacene in naphthalene crystals [1]. We further introduce a phase alternated protocol that extends the rotating-frame coherence time by an order of magnitude. These results establish pentacene-based molecular spins as a practical and high-performance platform for microwave quantum sensing, and the control techniques are broadly applicable to other molecular and solid-state spin systems.

We furhter demonstrate a sizable increase in the coherence time of a pentacene electronic spins by hyperpolarizing the proton spin bath. We leverage the high electron spin polarization of pentacene generated via optical excitation, enabling high nuclear spin bath polarization (> 60%) via dynamic nuclear polarization. The polarized nuclear spin bath provides a reduced magnetic noise environment, leading to enhanced electron spin coherence even under repeated triplet-state excitations [2]. These observations are supported by a theoretical model and cluster correlation expansion (CCE) simulations. Together, these results establish nuclear spin hyperpolarization as a practical and controllable route to engineering photo-addressable molecular qubit platforms.



Yifan Quan - University of Pennsylvania
231 S. 34 Street Philadelphia, PA, 19104 United States, Email: yquan@sas.upenn.edu

Paramagnetically Doped Metal–Organic Frameworks for Dynamic Nuclear Polarization: An EPR Study

Antareekshya Deka[1], Andreas Pöppl[1*]

[1]Felix-Bloch-Institute of Solid-State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, Linnéstrasse 5, Leipzig 04103, Germany
Email: antareekshya.deka@uni-leipzig.de

Metal-Organic frameworks (MOFs) have recently emerged as promising materials for gas storage and separation due to their high surface areas, high porosity, framework flexibility, etc[1,2]. MOFs are highly tunable porous materials with large surface areas, high porosity, and structural flexibility, enabling applications ranging from gas storage, separation, catalysis, etc [1,2]. Unlike rigid porous solids, many MOFs undergo dynamic structural transformations such as breathing, gate-opening, or swing effects in response to guest adsorption, temperature, or pressure [2-4].

In this work, Electron Paramagnetic Resonance (EPR) spectroscopy was employed to explore the gas adsorption behavior of well-known MOFs: YMOF-76, an activated yttrium metallic–organic framework of 1,3,5-benzenetricarboxylate [MOF-76(Y)]; ZIF-8 and ZIF-11, which are zinc-based zeolitic imidazolate frameworks. To gain insight into the local environment and host–guest interactions of the framework metal ions during gas adsorption, high-spin paramagnetic metal ions like Mn^{2}? (*S=5/2*) and Gd^{3}?(*S=7/2*) were introduced as spin probes into the MOF structure. These S-state ions, characterized by minimal orbital angular momentum, are particularly well-suited for Dynamic Nuclear Polarization (DNP) due to their suitable electron relaxation times and efficient polarization transfer, making them ideal candidates for hyperpolarization studies in solid-state NMR[5,6]. In addition, well-known DNP polarizing agents such as TEMPO and DPPH were confined within ZIF-11 and characterized by EPR spectroscopy to determine their incorporation sites within the pore structure and their dynamics. The insights gained from this research will provide a deeper understanding of MOFs doped with high spin metal ion centers and will also emphasize their potential for practical applications like gas adsorption, gas separation, and hyperpolarization techniques. Together, these approaches contribute to the establishment of MOFs as versatile platforms for probing framework dynamics and developing next-generation DNP strategies for hyperpolarization of adsorbed gases or guest molecules in porous materials.

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Antareekshya Deka - Felix Bloch Institute for Solid State Physics, Leipzig University Kirschbergstr.47, Wnr: 01.OG.mitte Leipzig, Saxony, 04159 Germany, Email: antareekshya.deka@uni-leipzig.de

200 **EPR Poster Session**

Enhancing the Stability of BDPA Radicals through Chemical Design and Synthesis

Olivia Woodward[1], Abigail Von Niederhausern[1], Hai Dang Nguyen[1], Yunfan Qiu[1]

Utah State University, Department of Chemistry and Biochemistry, Logan, UT 84322

The 1,3-bis(diphenylene)-2-phenylallyl (BDPA) radical is a well-studied carbon-based radical. Its abundant electron spin can be leveraged to polarize surrounding nuclear spins, making BDPA a widely used polarizing agent in dynamic nuclear polarization (DNP). However, its limited long-term stability remains a major challenge for extended studies and practical applications. In this project, sites of high spin density in BDPA were identified and targeted for chemical modification. Four sets of substituted BDPA derivatives were designed to enhance radical persistence by introducing bulky methyl and tert-butyl groups at key positions of radical delocalization, thereby limiting attack by reactive species. Computational studies showed that these substitutions reduced spin density at the targeted sites. After synthesis of the four BDPA derivatives and radical generation, degradation rates were measured using both UV-vis and EPR spectroscopy. These studies confirmed that the most highly substituted derivative exhibited greater stability than unmodified BDPA under identical conditions. These functionalized BDPA radicals provide new experimental opportunities for developing more persistent carbon-based radicals for future DNP applications.

Abigail Von Niederhausern - Utah State University
0900 Old Main Hill Logan, UT, 84322 United States, Email: abigailjvonn@gmail.com

Physics-Constrained AI Framework for Robust and Distortion-Tolerant EPR Oxygen Mapping

Adi Zehavi-Lenz[1], Irene Canavesi[2], Aharon Blank[3,4], Boris Epel[2,5], Mrignayani Kotecha[2], and Moti Freiman[1]

[1]Faculty of Biomedical Engineering, Technion - IIT, Haifa, Israel
[2]Oxygen Measurement Core, O2M Technologies, LLC, Chicago, IL 60612, USA
[3]Schulich Faculty of Chemistry, Technion - IIT, Haifa, Israel
[4]Scholl of Electrical and Computer Engineering, Tel Aviv University, Israel
[5]Department of Radiation and Cellular Oncology, The University of Chicago, IL 60637, USA

Electron paramagnetic resonance (EPR) imaging enables non-invasive quantitative oxygen (O2) mapping through relaxation–oxygen correlations, providing spatially resolved insight into tissue oxygenation, redox status, and microenvironmental heterogeneity[1,2]. However, accurate relaxation mapping remains limited by noise, spatial distortions arising from k-space acquisition inconsistencies, and instability in voxel-wise fitting, leading to substantial errors in estimated relaxation parameters (T1, T2). To address these challenges, we developed a physics-constrained AI framework for robust and distortion-tolerant estimation of relaxation parameters from spatial EPR imaging data. Our method enforces consistency with relaxation physics while learning spatial corrections for acquisition-induced distortions, suppressing fitting variability while preserving spatial structure. We evaluated our framework using experimental data from two complementary EPRI platforms: (i) a pulsed EPR microimaging system for high-resolution T2-based oxygen mapping[3], and (ii) JIVA-25 - an inversion recovery EPR imaging (IR-SPI) system developed by O2M company for T1-based oxygen quantification[4]. Datasets included controlled phantoms, enzyme-mediated reaction wells, and in-vivo kidneys measurements. Performance was assessed using normalized interquartile range (IQR/mean) and paired Wilcoxon tests on voxel-wise T1/T2 values, for significance of shift (bias) and significance of variability. All samples showed significant improvements in both shift and variability. For T2 mapping, the spread of T2 distributions was reduced by 48–56%, indicating enhanced robustness. For T1 mapping, voxel-wise variability decreased by ~67–100% in phantoms, ~19–82% in wells, and ~3–42% in in-vivo kidneys data, reflecting increasing physiological complexity while maintaining improved stability of parameter estimation. Overall, integrating physical signal models with AI framework enables distortion-tolerant and quantitatively stable EPR relaxation mapping, supporting reliable oxygen imaging in heterogeneous biological environments.

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Irene Canavesi - O2M Technologies, LLC
2201 W Campbell Park Dr. Chicago, IL, 60612 United States, Email: irene@oxygenimaging.com

Electron Paramagnetic Resonance Spectroscopy for Evaluation of Free-Radical Scavenging Properties: a Comparative Study of Ascorbic Acid and Ketone Bodies

Amarachi Emole[1] , Reef (Philip D, II) Morse [PhD][1]

1. Steppingstone MAgnetic Resonance Training (S.M.A.R.T) Center, Plymouth, Michigan, USA

Oxidative stress, a state of excess free radicals, has been implicated in several human diseases. Ketogenic diets have been postulated to reduce oxidative stress in neuropsychiatric disorders, but it is not clear how the antioxidant effect of ketogenic diets compare to established antioxidants like ascorbic acid (Vitamin C)[1,2] . Our study aims to evaluate the comparative effects of ketone bodies (acetoacetate and beta-hydroxybutyrate) and Vitamin C on free radical scavenging. Free radicals were produced using the Fenton reaction. Experiments were performed by adding antioxidants (10-100 mM), 5,5-dimethyl-1-pyrroline-N-oxide (DMPO, 100 mM) and ferrous sulfate to water. The reaction was started with hydrogen peroxide. The sample was placed in an EPR spectrometer to generate spectra representing the concentration of free radicals over time. Signal height was plotted over time to obtain the slope of the decay curve. At 10 mM, acetoacetate showed the fastest radical scavenging kinetics followed by beta-hydroxybutyrate and Vitamin C, with rate constants of 0.0024, 0.0004, and -0.0002 respectively. Scavenging rate was concentration dependent for most of the antioxidants, with the fastest scavenging rates noted at 20mM, except for Vitamin C which showed anomalous kinetics. Our study demonstrates that metabolic products from ketogenic diets have comparable or superior radical scavenging ability as Vitamin C. Currently, ketogenic diets are useful for treating drug-resistant childhood epilepsy[3], but future research should evaluate their effectiveness for many more disorders in which oxidative stress is implicated.

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Amarachi Emole - Steppingstone Magnetic Resonance Training (SMART) Center
650 Church St, UNIT 119 Plymouth, MI, 48170 United States, Email: amarachiemole22@gmail.com

Microwave phase noise mitigation using double quantum coherent control of NV-centers in diamond

Amilcar Jerónimo Pérez,[1,2] Janis Smith,[1,2] Yaser Silani,[1,2] Maziar S. Ziabari,[1,2] Andris Berzins,[1,2] Maxwell D. Aiello,[1,2] Bryan A. Richards,[1,2] Donald Ferschweiler,[1,2] Victor M. Acosta.[1,2]

University of New Mexico, Department of Physics and Astronomy, Albuquerque, NM USAUniversity of New Mexico, Center of High Technology Materials(CHTM), Albuquerque, NM USA

Nitrogen vacancy (NV) centers in diamond are becoming an attractive sensing platform for applications in magnetoencephalography (MEG), nuclear magnetic resonance (NMR) spectroscopy, and the search for new spin dependent interactions in particle physics experiments. However, to achieve femtotesla level magnetic field sensitivity, a practical challenge on the NV sensor is microwave phase noise.[1] In this work, we propose that by taking advantage of the full spin-1 property of the NV center, and by driving both spin transitions $m_s = 0$ « $m_s=+1$ and $m_s = 0$ « $m_s=-1$ with the same microwave generator, the effect of microwave phase noise can be mitigated.

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Amilcar Jerónimo Pérez - University of New Mexico
Department of Physics and Astronomy MSC07 4220 Albuquerque, NM, 87131 United States, Email: ajeronimo75@unm.edu

Confining Molecular Spin Qubits in Two-Dimensional Solid-State Architectures

Anna Champ,[1] Eleanor Mackintosh,[1] André Koch Liston,[1] Sanghyo Lee,[2] Eric D. Walter,[3] Raphaël P. Hermann,[4] Augustin Braun,[1] Willa Mihalyi-Koch,[1] Jeffrey M. McNeill,[1] Daniel G. Chica,[1] Johan van Tol,[5] Tomas Orlando,[5] Mykhaylo Ozerov,[5] Byeongjun Gil,[2] Myung-Geun Han,[2] Jonathan S. Owen,[1] Timothy C. Berkelbach,[1] Milan Delor,[1] Michael L. Steigerwald,[1] Colin Nuckolls,[1] Xavier Roy,[1] Arun Ramanathan[1]

1. Columbia University, Department of Chemistry, New York, NY 10027, USA
2. Brookhaven National Laboratory, Condensed Matter Physics &; Materials Science, Upton, NY 11973, USA
3. Pacific Northwest National Laboratory, Environmental Molecular Sciences Laboratory, Richland, Washington 99352, USA
4. Oak Ridge National Laboratory, Materials Science and Technology Division, Oak Ridge, TN 37831, USA
5. National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA

Molecular spin qubits (MSQs) offer a chemically tunable platform for quantum sensing and information processing, yet their integration into solid-state environments remains limited by rapid decoherence induced by surface interactions and environmental noise.[1] Here, we introduce van der Waals (vdW) confinement within layered two-dimensional materials as a general strategy to stabilize and enhance coherence in MSQs. Using reductive intercalation, we confine cobaltocene ($CoCp_2$) molecules within the vdW gaps of diamagnetic semiconductors SnS_2 and $CdPS_3$, forming self-assembled mixed-valence superlattices in which a subset of $^{59}Co^{2+}$ centers act as addressable S = 1/2 qubits. Comprehensive structural and spectroscopic characterization confirms successful confinement, charge transfer, and preservation of the host lattice framework. Continuous-wave electron paramagnetic resonance (EPR) measurements show that confinement dramatically alters the electronic structure of CoCp2, indicating substantial reorganization of its local electronic environment within the vdW gap. Probing the spin dynamics with pulsed EPR methods, we observe an increase in spin-lattice relaxation time (T_1) by three orders of magnitude compared to molecular crystals, along with measurable signals up to 100 K. The phase memory (T_m) of vdW confined molecules shows similar substantial enhancement, but only a weak temperature dependence as it traces T_1 with measurable echo up to 100 K, above which T_m is limited by T_1. We attribute the enhanced coherence upon confinement to the increased Jahn-Teller distortion due to non-covalent interactions between the host and the guest. These results establish vdW confinement as a powerful design strategy for engineering spin coherence in molecular systems, providing a pathway toward atomically precise, scalable quantum sensing hybrid architectures with deterministic placement and controlled orientation of MSQs.

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Anna Champ - Columbia University
3000 Broadway New York, New York, 10027 United States, Email: aec2262@columbia.edu

Applications of EPR to Biopharma: Structure, Dynamics, and Equilibria of a Monomer-Dimer System by Pulsed Dipolar Spectroscopy

Austin R. Gamble Jarvi[1]

High Q Technologies, Waterloo, ON, Canada

Pulsed Dipolar Spectroscopy (PDS), a branch of Electron Paramagnetic Resonance (EPR) spectroscopy that focuses on the measurement of interspin dipolar interactions, holds significant value for the investigation of protein-protein interactions (PPIs), capable of elucidating structural constraints, determining dynamic information, and counting coupled spins. Protein oligomerization is a specific type of PPI of great interest to pharmaceutical and drug-discovery industries. Because oligomerization influences and regulates many key protein categories such as enzymes, ion channels, and transcription factors, it plays a vital role in many biological and physiological processes that make appealing targets for therapeutic development. Therefore, understanding the mechanism of interaction is of significant interest to the scientific community.

Here, we apply Double Electron Electron Resonance (DEER), a robust and popular PDS technique, to investigate the dimerization of a homodimeric protein system. The distance distributions extracted from the DEER data are used to gain insight into the structure and dynamics of the dimeric complex, while careful analysis of the modulation depth of the dipolar traces reveals the populations of monomer and dimer states. Furthermore, we investigate the changes in these aspects as a function of buffer conditions and against the introduction of compounds that promote dimerization of the protein. These findings exemplify the capacity of EPR to contribute to questions across the PPI space, and the principles demonstrated here can be easily extrapolated toward other hot-topics within the biopharmaceutical industry, such as induced proximity and targeted protein degradation.

Austin Gamble Jarvi - High Q Technologies
485 Wes Graham Way Waterloo, Ontario, N2L0A7 Canada, Email: austin.gamblejarvi@highqtechnologies.com

High Spatial Resolution Quantitative Oxygen Imaging Using Image Domain Averaging

Boris Epel[1,2], Irene Canavesi[1], and Mrignayani Kotecha[1]

[1] Oxygen Measurement Core, O2M Technologies, LLC, 2201 W Campbell Park Dr., Chicago, IL 60612, USA
[2]Department of Radiation and Cellular Oncology, The University of Chicago, Chicago, IL 60637, USA

Oxygen is central to metabolic activity, growth, reproduction, disease, and recovery pathways across all pathologies. Electron paramagnetic resonance oxygen imaging (EPROI) has emerged as the leading technique to image partial oxygen pressure (pO_2) maps in vitro and in vivo. The current gold standard for pO_2mapping using EPROI is inversion recovery electron spin echo (IRESE) with a radial acquisition scheme, which is fast, provides high pO_2 resolution, but suffers from lower spatial resolution. The other method, single point imaging (SPI), provides higher spatial resolution, but suffers from lower signal-to-noise ratio (SNR) and lower pO_2 resolution for T_2* imaging methodologies. In this work, we present advanced inversion recovery single point imaging (AIR-SPI) that overcomes the SNR limitations of SPI and provides T_1-based pO_2 maps with high pO_2 and high spatial resolution. In addition, AIR-SPI has lower power deposition due to being a free-induction decay (FID)-based method instead of an echo-based method. The AIR-SPI method is demonstrated in phantoms and mouse tumor images.

Boris Epel - O2M Technologies, LLC
2201 W Campbell Park Ave Chicago, IL, 60612 United States, Email: boris.epel@oxygenimaging.com

Measurement of TEMPO Reduction to Determine Storage Effects on Antioxidant Levels in Fruits and Vegetables III

Emily D. Cheng[1,2], Reef (Philip D., II) Morse[2]

1. Washtenaw Community College, 4800 E Huron River Dr., Ann Arbor, MI 48105
2. Steppingstone Magnetic Resonance Training Center, 650 Church Street Suite 110A, Plymouth, MI 48170

In our previous experiments, EPR (Electron Paramagnetic Resonance) was used to measure the reduction rate of TEMPO (2,2,6,6-tetramethylpiperidine-N-oxyl), a free radical, in various fruit and vegetable solutions with the goal of measuring antioxidant activity.[1,2] This poster updates those results. As previously, first-order rate constants were calculated from the height of the central line, and any differences between fresh and frozen samples were noted. Additionally, we collected full spectra for some samples with the intent of measuring rotational correlation times of the nitroxide (TEMPO) in the sample over time. These results show that antioxidant levels in frozen samples were (except for asparagus and raspberries) lower than in fresh samples. The average first-order rate constant of frozen blueberry samples was $1.73 \times 10^{-5} s^{-1}$, as opposed to the $1.34 \times 10^{-4} s^{-1}$ of fresh blueberry samples. The average rate constants of other frozen samples compared to their fresh counterparts were $1.19 \times 10^{-5} s^{-1}$ compared to $4.82 \times 10^{-5} s^{-1}$ for blackberry samples, $2.25 \times 10^{-4} s^{-1}$ compared to $1.17 \times 10^{-3} s^{-1}$ for spinach samples, $5.83 \times 10^{-4} s^{-1}$ compared to $3.20 \times 10^{-4} s^{-1}$ for asparagus samples, and $6.42 \times 10^{-4} s^{-1}$ compared to $6.64 \times 10^{-4} s^{-1}$ for raspberry samples. To our surprise, the rotational correlation times of the nitroxide in various samples change with time, and we are currently gathering more data to verify this observation.

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Emily Cheng - University of Michigan
3132 Cherry Tree Ln Ann Arbor, MI, 48108 United States, Email: emilydcheng@gmail.com

Improving the modulation in 4-pulse DEER with swept observer pulses

Eric R. Lowe[1], Stefan Stoll[2], Jason P. Kestner[1]

University of Maryland Baltimore County, Department of Physics, Baltimore, MD 21250University of Washington, Department of Chemistry, Seattle, WA 98195

Swept pump pulses are known to improve DEER modulation depth by exciting a larger fraction of the spin label spectrum.[1] Here we extend the idea to the observer side, replacing the narrowband observer pulses of the 4-pulse DEER sequence with frequency-swept pulses, using a composite pulse sequence to prevent phase dispersion. Optimal pulse shapes for the swept observer pulse sequence are obtained by numerical maximization of the modulation-to-noise ratio (MNR), explicitly accounting for the microwave resonator transfer function and microwave power limitations. We benchmark the new approach for nitroxide-nitroxide and Cu(II)-Cu(II) DEER against Gaussian observer pulses, with both pulse shapes optimized under the same constraints. We find that the improvement for nitroxides is marginal. However, for the much broader Cu(II) spectrum, we see a 45% improvement in MNR, indicating that swept observer excitation is most beneficial for broadband spectra.

Eric Lowe - University of Maryland, Baltimore County
7830 Paragon Circle, Apt 411 Elkridge, Maryland, 21075 United States, Email: elowe2@umbc.edu

Dual EPR spin probe and label approach resolves origins of protein and coupled solvent dynamics and confinement-induced folding in fibrillar amyloid-ß(1-42)

Hana Alsheikh,[1] Katie L. Whitcomb,[1] and Kurt Warncke.[1]

Emory University, Department of Physics, Atlanta, GA 30322-2430

Monomeric amyloid-ß (Aß) is an intrinsically disordered protein (IDP), with common lengths of 38-42 residues. Aß forms fibrils with characteristic amyloid cross-ß sheet structure and a disordered N-terminal region (residues 1-17).[1] To gain insight into molecular mechanisms of Aß function and dysfunction in Alzheimer's disease, a dual spin probe and spin label electron paramagnetic resonance (EPR) spectroscopy approach is applied in a frozen solution system,[2,3] that features temperature (*T*) -controlled, ice-boundary confinement. Protein and coupled solvent dynamical properties of Aß42 fibrils are addressed by using the spin-probe, TEMPOL, colocalized with the protein. Spin-labelling with Cu^{2+} at native His6, 13, 14 is used to assess the N-terminal domain dynamics.[4,5] Temperature-dependence (220-265 K) of TEMPOL rotational mobility resolves two correlation times, denoted "fast" (dynamically disordered region) and "slow" (hydration region), with normalized weights, W_f and W_s. The overall decrease in W_f with increasing confinement proceeds in three stages: compaction 1 (C1) - structure consolidation (SC) - compaction 2 (C2). This behaviour is also characterized in fibrils and oligomers of the IDP, a-synuclein.[6] From the Cu^{2+} label perspective, the arrest of Cu^{2+} mobility with decreasing *T* indicates N-terminal domain collapse as the primary C1 origin. Cu^{2+} binding maintains the TEMPOL-detected three-stage compaction but increases C1 extent and shifts SC to lower *T*. These results are consistent with bound Cu^{2+} promotion of N-terminal region disorder. A thermodynamic treatment of the three-stage compaction mechanism provides an approach to quantitative assessment of Aß42–drug interactions. Supported by NIH R01 GM142113.

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Hana Alsheikh - Emory University
400 Dowman Dr Atlanta, Georgia, 30322 United States, Email: halshei@emory.edu

Applied EPR for degradation mechanisms of per-and polyfluoroalkyl substances (PFAS): A scoping review

Isaac Spackman, Shubham Vyas

Colorado School of Mines, Department of Chemistry and Geochemistry, Golden, CO 80401

Adverse health effects due to exposure to per- and polyfluorinated 'forever chemicals' are estimated to cost more than $5 billion dollars yearly in the US alone, yet the cost to remove these persistent pollutants is estimated in *trillions* of dollars. Current remediation technologies are limited by both the costs of separation and primary energy costs resulting in few cases of economically viable scaling. These limitations have led to increased efforts to understand the fundamental chemical mechanisms at play in PFAS degradation to identify more energy efficient degradation strategies.

Many diverse decontamination strategies are thought to proceed through a series paramagnetic fluoroalkyl radical intermediates facilitated by reactive oxygen species or aqueous electrons, yet the fluoroalkyl radical intermediates common to these pathways have not been experimentally observed. The reason for this gap in evidence is currently unclear; the lifetimes of these intermediates are largely unknown and may not be sufficiently long to be observed via EPR. If the species are sufficiently long lived, rapid spin relaxation in the aqueous environment may also limit detection ability. Furthermore, commonly used experimental conditions and instrument settings might fundamentally preclude observation of these intermediates even if they were sufficiently long lived and had appropriate spin relaxation rates.

To clarify the extent of the evidence supporting such mechanisms, we present a scoping review focused on the use of EPR spectroscopy in PFAS degradation studies. Specifically, we aim to (1) describe the range of paramagnetic species that have been detected in PFAS degradation studies and (2) quantitatively evaluate the experimental conditions under which these species have been observed including pH ranges, reactant concentrations and critical spectrometer parameters. Finally, we present a qualitative analysis of the purpose and context in which EPR has been used for mechanistic studies of PFAS degradation, highlighting several ambiguities and misinterpretations in the literature.

Isaac Spackman - Colorado School of Mines
1500 Illinois St Golden, CO, 80401 United States, Email: ispackman@mines.edu

Ex Vivo Liver Electron Paramagnetic Resonance Oxygen Imaging for Optimization of Organ Preservation Time

Irene Canavesi[1], Casie Pandexter[2], Boris Epel[1,3], Basak E. Uygun[2], and Mrignayani Kotecha[1]

[1] Oxygen Measurement Core, O2M Technologies, LLC, 2201 W Campbell Park Dr., Chicago, IL 60612, USA
[2]Center for Engineering in Medicine and Surgery, Massachusetts General Hospital, Harvard Medical School, Boston, MA 02114, USA
[3]Department of Radiation and Cellular Oncology, The University of Chicago, Chicago, IL 60637, USA

Orthotopic organ transplantation remains the only viable method for treating end-stage organ diseases. Current preservation times for whole organs are limited to only a few hours of storage, resulting in inefficient use of available critical organs [1-3]. Since organ preservation is a multi-step process, potentially damaging to the organ, the non-invasive assessment for viability and function is important to optimize the preservation methods and increase the storage time. Trityl-OXO71-based electron paramagnetic resonance oxygen imaging (EPROI) is the only method that provides partial oxygen pressure (pO_2) maps that can be used to assess cell and organ viability [4,5]. In this study, ex vivo mouse liver pO_2 maps were acquired for three groups of livers (n = 4 each, 2 males and 2 females) in a petri dish: fresh, 48 hours post static cold storage (SCS) (48h-SCS), and 72 hours post SCS (72h-SCS). The pO_2 measurements were performed using the inversion recovery electron spin echo (IRESE) sequence[6]. The experiment included 90 minutes of continuous pO_2 imaging while perfusing the livers with 100% oxygenated media, 1 hour of warm ischemia (WI) period simulating the typical cutoff time for transplant organs, then another 90 minutes of pO_2 imaging again with perfusion of 100% oxygenated media to the livers. Mean pO_2 was calculated by masking the liver boundaries using the signal amplitude maps as well as pictures. A statistical difference between pre- and post-WI pO_2 was found for 48h-SCS and 72h-SCS groups (p-value < 0.0001), but not for fresh livers. A comparison between the three groups showed a statistical difference after WI between fresh-48h-SCS and fresh-72h-SCS, but not before WI, suggesting that livers from all groups were initially viable, but the 48h-SCS and 72h SCS groups did not survive the WI time. It was also found that more than 30% of voxels in the livers are hypoxic (pO_2 < 10 torr) in pre-WI time, indicating a high cellular oxygen consumption, but also exposure to hypoxic extracellular space. This is the first study, to the best of our knowledge, where EPROI is utilized to assess organ viability for transplantation.

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Irene Canavesi - O2M Technologies, LLC
2201 W Campbell Park Dr. Chicago, IL, 60612 United States, Email: irene@oxygenimaging.com

High field microfluidic NMR spectroscopy by longitudinal magnetization detection with pulsed NV magnetometry

Janis Smits[1], Bryan Richards[1], Yaser Silani[2], Andrew McDowell[3], Andrey Jarmola[4], Victor Acosta[1]

Center for High Technology Materials, University of New Mexico, Albuquerque, New Mexico, United StatesDepartment of Electrical and Computer Engineering, University of Washington, Seattle, Washington NuevoMR, Albuquerque, NM, USA ODMR Technologies Inc., El Cerrito, CA

The power of NMR spectroscopy as a quantitative analysis tool across multiple disciplines has been well established. Its main drawback is a relatively poor sensitivity when compared to mass-spectrometry, especially in scenarios where the analyte concentrations and volumes are small. This is almost always the case in fields such as metabolomics, which has prompted the development of magnet systems that can produce higher field and microcoils capable of detecting smaller quantities of analyte.
The nitrogen-vacancy (NV) center in diamond can be a strong competitor to NMR microcoils when performing NMR spectroscopy on small volumes (<1nL). The sensor is optically addressed which enables magnetometry at the optical diffraction limit thus being a natural fit for small volume NMR. Here we present some preliminary work showing NV NMR spectra at a moderate field of ~0.5 T using a Ramsey-ENDOR protocol. The magnetometer itself has a photon shot-noise limited magnetic sensitivity of ~5pT?$s^{1/2}$ which equates to a proton molar sensitivity of ~ 12M for an SNR of 3 at a bias field of 0.5 T. These results build on previous published work[1] showing using the Ramsey-M_z protocol, with the key improvement being the more than an order-of-magnitude improvement in magnetic sensitivity achieved by using a Hahn-Echo measurement on the NVs to read out the nuclear magnetization signal.

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Janis Smits - University of New Mexico
1313 Goddard st SE Albuquerque, New Mexico, 87106 United States, Email: smitsjanis@gmail.com

Structural Characterization of the Cu(II)-NTA Spin Label on a-Helices by Electron Paramagnetic Resonance and X-ray Crystallography.

Joerg Reichenwallner,[1] Jessica E. Besaw,[1] Oliver P. Ernst[1,2]

1. University of Toronto, Department of Biochemistry, Toronto, ON, M5S 1A8, Canada.
2. University of Toronto, Department of Molecular Genetics, Toronto, ON, M5S 1A8, Canada.

Compared to the classical nitroxide-based studies, Cu(II) ions have been demonstrated to constitute excellent alternative candidates for site-directed spin-labelling in pulsed electron paramagnetic resonance (EPR). Particularly, the Cu(II)-nitrilotriacetic acid (NTA) spin label in combination with helix-based double histidine (dHis) mutations at positions *i* and *i*+4 provides non-covalent assemblies that are capable of providing high fidelity distance information to resolve subtle conformational changes in biological macromolecules.[1] Here we present first atomic-resolution X-ray crystal structures of the rigid octahedral coordination in the chelated dHis-Cu(II)-NTA complex.[2] A comparison of crystal structure-derived intra-molecular distances with pulsed EPR results from T4 lysozyme revealed remarkable distance agreement. Besides that, we were also able to identify the origins of proper Cu(II)-NTA binding as well as non-conventional binding modes. The rigid octahedral binding modes could be generally linked to low micromolar binding affinities. This study provides a wealth of geometric constraints that can be leveraged in modelling and molecular dynamics programs to extract, understand and accurately predict structural details in proteins from EPR experiments. Altogether, those findings allow for setting up further guidelines for dHis site selection in structural investigations of proteins.
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Joerg Reichenwallner - University of Toronto
1 King's College Circle, Medical Sciences Building Toronto, ON, M5S 1A8 Canada, Email: joerg.reichenwallner@utoronto.ca

Exploring Matter Through Electron Spin Resonance: Tools and Opportunities at the NHMFL

Johan van Tol, Jurek Krzystek, Andrew Ozarowski, Tomas Orlando, Stephen Hill

National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310

The Electron Magnetic Resonance (EMR) program at the National High Magnetic Field Laboratory provides researchers with access to state-of-the-art electron spin resonance (ESR/EPR) instrumentation spanning a wide range of frequencies, magnetic fields, temperatures, and experimental modalities. These capabilities enable investigations of electronic structure, magnetic interactions, spin dynamics, defects, radicals, transition-metal complexes, quantum materials, biological systems, and other spin-dependent phenomena that are inaccessible using conventional laboratory-scale instrumentation.

As a national user facility, the EMR program supports a diverse scientific community through access to unique high-field and high-frequency ESR resources, expert technical guidance, collaborative opportunities, and user training. Measurements can be performed across a broad range of experimental conditions, allowing researchers to address challenging questions in chemistry, physics, materials science, engineering, and the life sciences.

Here we provide an overview of the EMR program's instrumentation, experimental capabilities, and user access model. Representative applications and recent scientific highlights illustrate how advanced ESR techniques at the National High Magnetic Field Laboratory can provide unique insights into the structure and dynamics of paramagnetic systems and support cutting-edge interdisciplinary research.

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Johan van Tol -
1800 E Paul Dirac Dr Tallahassee, Florida, 32310 United States, Email: vantol@magnet.fsu.edu

Elucidating Electronic Structure and Relaxation Pathways of Transition Metal Qubits via High Power EPR Spectroscopy

Kavipriya Thangavel,[1] Dipanti Borah,[2] Vignesh Kasi,[2] Maheswaran Shanmugam,[2] Andreas Pöppl[3], Stephen Hill[1,4,5]

National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USADepartment of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076, IndiaFelix Bloch Institute of Solid State Physics, University of Leipzig, 04103 Leipzig, GermanyDepartment of Physics, Florida State University, Tallahassee, FL 32306, USADepartment of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306, USA

Molecular spin qubits, known for their precise control, scalability, tunability, and room-temperature capability to sustain multiple quantum states, are promising candidates for quantum information science [1]. These systems enable large-scale production, precise tuning of spin environments, and arrangement into 2D or 3D lattices. Progress in their design and integration is crucial for overcoming challenges related to addressability, coherence, and scalability in future quantum technologies. In this context, metal–organic frameworks (MOFs) have recently gained attention as tunable platforms for molecular qubits. Among them, the breathing MOF MIL-53 [2] has emerged as a promising material for quantum information science applications [3].
In this context, we performed high-field continuous-wave (CW) electron paramagnetic resonance (EPR) experiments up to 413 GHz on Co(II)-based metal complexes and a Cr(III)-based MOF to probe their electronic and structural properties. Two low-spin Co(II) (S = 1/2) complexes, [CoCl(DPPE)2]SnCl3, with square pyramidal (Co-SP) and trigonal bipyramidal (Co-TBP) geometries, exhibited distinct EPR signatures arising from their different coordination environments. High-power W-band EPR (HiPER) measurements further revealed temperature-dependent relaxation behavior up to 60 K. At 5 K, Co-TBP showed $T2$ ˜ 5.8 µs and $T1$ ˜ 0.62 ms, while Co-SP exhibited $T2$ ˜ 3.5 µs and $T1$ ˜ 0.98 ms. For MIL-53, $T2$ and $T1$ were approximately 0.96 µs and 50 µs, respectively, at 5 K. Furthermore, field-dependent relaxation measurements covering the S = 3/2 spectral features, together with field-dependent ELDOR-detected nuclear magnetic resonance (EDNMR) experiments, were performed to elucidate the relaxation behavior of different transitions and probe the surrounding nuclear spins, respectively.

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Kavipriya Thangavel - National high Magnetic Field Laboratory
1800 E Paul Dirac Dr, Tallahassee, Florida, 32310 United States, Email: kt24@fsu.edu

L-band (1.0 GHz) Rapid-Scan EPR Spectroscopy and Imaging with a Surface Coil Resonator

Liberty Debrah,[1] Tanden Hovey,[1] Georgina Amassah, Hanan Elajaili,[2] Eva S. Nozik,[2] Sandra S. Eaton,[1] and Gareth R. Eaton[1]

[1]Department of Chemistry and Biochemistry, University of Denver, Denver, CO 80210
[2]Cardiovascular Pulmonary Research Laboratories and Pediatric Critical Care Medicine, University of Colorado Anschutz Medical Campus, Aurora, CO 80045

1 GHz (L-band) provides a workable balance between penetration depth and signal-to-noise ratio for EPR preclinical studies of mice. The many options for synthesis of nitroxide radicals permit design of probes for specific applications, although the faster relaxation times of nitroxides than of trityl radicals make them less well suited for pulsed EPR. Rapid scan EPR, which is well suited for the relaxation times of nitroxides, is implemented in our recently-characterized spectrometer.[1] Surface coil resonators permit localized study of radicals in objects that are larger than can be accommodated conveniently in volume resonators.[2]The use of the L-band spectrometer with a 10 mm surface coil to characterize depth of penetration and the principle of reciprocity, for imaging, and to acquire spectra of trapped radicals in wounds on the skin of mice will be discussed.

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Liberty Debrah - University of Denver
Dept of Chemistry and Biochemistry, 2101 E. Wesley Ave Denver, CO, 80210 United States, Email: liberty.debrah@du.edu

Probing Intermolecular Exchange Weak Interactions from Single Crystal HFEPR Measurements

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

1. Central European Institute of Technology, Brno University of Technology, Brno, 61200, Czechia.
2. Departamento de Física, Facultad de Bioquímica y Ciencias Biológicas, Universidad Nacional del Litoral (UNL), 3000 Santa Fe, Argentina.

Molecules with a spin array exhibit properties highly relevant for emerging quantum technologies, including quantum bits (qubits) for quantum computation.[1,2] Advances in continuous-wave High-frequency electron paramagnetic resonance (HFEPR) allow new opportunities to access to describe the spin dynamics, magnetic anisotropy, and spin-spin interactions (exchange interaction) in potential qubits such as transition metal coordination compounds. Additionally, weakly coupled spin chains have been discussed as potential wired up qubit systems.[3] Here we investigate a dinuclear Cu(salen) complex in which each Cu(II) center carries spin S = ½ in powder and single crystal samples. The system consists of magnetically inequivalent molecules related by a 180° rotation about the *b* axis, forming weakly coupled layers within the crystal structure. In this work, HFEPR is employed to probe different dynamic regimes of the compound arising from intermolecular exchange weak interactions. EPR powder spectra of Cu(salen) recorded at 9.5 GHz, 95 GHz, and 397 GHz at room temperature show that increasing the excitation frequency significantly modifies the spectral profile, enabling access to different dynamic regimes (merged and split) supported by the weak intermolecular exchange interactions in the array. This interaction translates into additional peaks (U-peaks) associated with each dynamic phase.[2] To better understand this behavior, angular-dependent HFEPR measurements on an oriented single crystal were performed, providing detailed information on magnetic anisotropy and spin dynamics. With these results, attention is given to a regime of collapsed EPR peaks exhibiting strong linewidth narrowing, which suggests enhanced spin coherence and potential relevance for molecular qubit applications.

Luan Lima - Brno University of Technology (BUT)
Uprkova 1576/1 Brno, South Moravia, 62100 Czech Republic, Email: 272343@vutbr.cz

Insights into Second-Shell Waters of Gadolinium Contrast Agents using Electron-Nuclear Double Resonance (ENDOR): Implications for Relaxivity and Dynamic Nuclear Polarization

Martyna Judd,[1] Peter E. Doan,[1] Matthew D. Bailey,[1] Thomas J. Meade,[1] Brian M. Hoffman,[1] Songi Han.[1]

[1]Northwestern University, Department of Chemistry, Evanston, IL, 60208, USA

Water molecules in the second coordination sphere of Gd^{3+} contrast agents modulate proton relaxivity.[1] However, their organization, dynamics, and quantitative contribution remain poorly constrained and difficult to untangle from inner- and outer-sphere water dynamics. Conventional relaxometry approaches e.g. nuclear magnetic relaxation dispersion, rely on model-dependent interpretations[1,2] that can become murky when contending with heterogeneous or transient hydration environments. Hence, key parameters governing water exchange, hydrogen-bonding networks, and outer-sphere contributions remain difficult to validate experimentally. Electron paramagnetic resonance (EPR) methods are typically used to constrain the contributions of paramagnetic rotational correlation and spin-lattice relaxation times to the overall water relaxivity mechanism.[2,3] Here, we extend EPR methods to investigate second-shell water interactions in Gd^{3+} complexes, using ^{1}H and ^{2}H electron–nuclear double resonance (ENDOR) spectroscopy at 2 K. ENDOR directly probes the hyperfine coupling distribution in the sample, and therefore the distribution of coordination dynamics. Additionally, by detecting only on the |-7/2> to |-5/2> Gd^{3+} transition we can probe first vs. second-shell water populations in isolation, allowing their spatial and dynamic characteristics to be distinguished. Finally, we explore how the tethering of Gd^{3+} contrast agents to nanodiamond surfaces – which has been shown to give 10-fold relaxivity enhancement[4] – impacts the hydration shell. Critically, there is limited understanding behind this enhancement and whether water confinement and surface interactions play a role. We use ENDOR to model the hydration dynamics in these systems, and additionally explore the potential of resonance matching between nanodiamond P1-centers and Gd^{3+} as a way to enhance dynamic nuclear polarization efficiency at ambient temperature.

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Martyna Judd - Northwestern University
2170 Campus Drive, Silverman 4560 Evanston, IL, 60208 United States, Email: martyna.judd@northwestern.edu

Rabi Beat Spectroscopy of Spins Undergoing Fast Exchange

Michael K. Bowman

University of Alabama, Department of Chemistry and Biochemistry, Tuscaloosa, AL 35487

Rabi Beats are driven oscillations used to manipulate spins and entangled states in quantum information applications. Rabi Beats also expose properties of the spin system that are not available in the spin Hamiltonian approximation for CW EPR spectroscopy. The CW spectrum of a rapidly-exchanging solution of spins after collapse into a one-line is completely described by one or two complex eigenvalues. However, Rabi Beats reveal at least six eigenfunctions/ eigenvalues while the microwave driving field is applied. These eigenvalues control the state of the system after application of the strong driving field. A spin system whose spectrum has exchange-collapsed to a single line is used to reveal the involvement of multiple eigenstates over a range of driving fields.

Michael Bowman - The University of Alabama
Box 870336 Tuscaloosa, Alabama, 35487-0336 United States, Email: mkbowman@ua.edu

Polarization-Controlled Floquet Transitions in Strongly Driven Electron Spin Pairs

N. C. Pak[1], S. I. Atwood[1], P. Poudel[1], B. A. Odeke[1], A. Ahmad[1],C. Nuibe[1],V. V. Mkhitaryan[2], J. M. Lupton[2], R. M. Stolley[3], and C. Boehme[1]

[1]Department of Physics &; Astronomy, University of Utah, Salt Lake City, UT, USA
[2]Institute of Experimental and Applied Physics and Halle-Berlin-Regensburg Cluster of Excellence CCE, University of Regensburg, 93053 Regensburg, Germany
[3]Department of Chemistry, University of Utah, Salt Lake City, UT, USA

The interaction of periodically driven quantum systems with strong oscillating fields gives rise to Floquet states whose properties can differ fundamentally from those observed in the weak-driving regime[1–3]. While multiphoton magnetic resonance transitions have been extensively investigated, the role of the resonant drive-field's linear polarization direction relative to the static magnetic field B_0 in controlling Floquet-state symmetry and the associated transition selection rules has received comparatively little experimental attention[4-6]. Here, we investigate polarization-dependent Floquet transitions in weakly coupled electron spin pairs using electrically detected magnetic resonance (EDMR) of spin-dependent electron-hole polaron pair recombination current in a bipolar injection devices with the fully (per-) deuterated p-conjugated polymer poly[2-methoxy-5-(2'-ethylhexyloxy)-p-phenylene vinylene] (d-MEH-PPV) under strong drive conditions. Room-temperature measurements were performed over a broad range of drive field amplitudes B_1, extending into the regime where B_1 approaches B_0. By continuously varying the orientation of the oscillating magnetic field with respect to the direction of B_0, pronounced and systematic changes in the electrically detected resonance spectra are observed. The relative intensities of one-, two-, and three-photon transitions exhibit a strong dependence on the polarization direction, while an additional resonance is identified as a four-photon transition through quantitative agreement with Floquet calculations. Numerical simulations based on Floquet theory reproduce both the resonance positions and their polarization dependence, demonstrating that drive-field polarization modifies the symmetry of the driven spin Hamiltonian and thereby controls the selection rules governing multiphoton transitions,[5,6]. These results establish drive field polarization as a powerful experimental parameter for engineering Floquet spin dynamics and provide new insight into spin-dependent transport processes in strongly driven electron-spin systems, with potential applications in coherent spin manipulation and quantum information science.

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Nathan Chanhyun Pak - University of Utah
270 S 1400 E Salt Lake City, UT, 84092 United States, Email: u1149154@utah.edu

Navigating the Challenges of Excitation: Modeling Orientationally Selective Pulsed Dipolar EPR.

Nicholas A. Moriglioni,[1] Yannik Limbach,[2] Hassane El Mkami,[3] Katrin Ackermann,[2] Robert I. Hunter,[3] Graham M. Smith,[3] Bela E. Bode,[2] Sunil Saxena[1]

University of Pittsburgh, Department of Chemistry, Pittsburgh, PA 15260, U.S.A.University of St Andrews, School of Chemistry, St Andrews KY16 9ST, Scotland, U.K.SUPA, University of St Andrews, School of Physics and Astronomy, St Andrews KY16 9SS, U.K

Pulsed dipolar EPR spectroscopy has become a powerful tool for nanometer-scale distance measurements in biophysics. The combination of rigid spin labels, such as Cu(II)-NTA, with high-frequency EPR offers enhanced sensitivity and precise structural insight. However, these measurements are often limited by excitation bandwidth. With rigid spin labels, selective excitation may result in orientational selectivity, complicating data acquisition and analysis. As a remedy we have developed a model system which investigates acquisition schemes to obtain an orientationally averaged signal in as few experiments as possible. This method debuted in our work with DEER on the Cu(II)-NTA spin label at Q-Band.[1-3] Since then, we have developed the model to simulate both DEER and RIDME experiments at X-, Q-, and W-band. We've recently applied this model to find the optimal acquisition scheme for RIDME on Cu(II)-NTA at W-band (~95 GHz). We found that only four magnetic field positions are necessary to achieve an orientationally averaged signal despite excitation of only ~0.43% of the spin population. This framework provides an efficient means to overcome excitation limitations by finding optimal field positions informed by simulated PD-EPR. We expect the application of the model to be broadly applicable to high-field pulsed EPR studies with rigid spin labels. Supported by NSF BSF MCB 2407706.

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Nicholas Moriglioni - University of Pittsburgh
219 Parkman Ave. Pittsburgh, PA, 15213 United States, Email: nam253@pitt.edu

Enhancing the Stability of BDPA Radicals through Chemical Design and Synthesis

Olivia Woodward[1], Abigail Von Niederhausern[1], Hai Dang Nguyen[1], and Yunfan Qiu[1].

Utah State University, Department of Chemistry and Biochemistry, Logan, UT 84322

The 1,3-bis(diphenylene)-2-phenylallyl (BDPA) radical is a well-studied carbon-based radical. Its abundant electron spin can be leveraged to polarize surrounding nuclear spins, making BDPA a widely used polarizing agent in dynamic nuclear polarization (DNP). However, its limited long-term stability remains a major challenge for extended studies and practical applications. In this project, sites of high spin density in BDPA were identified and targeted for chemical modification. Four sets of substituted BDPA derivatives were designed to enhance radical persistence by introducing bulky methyl and tert-butyl groups at key positions of radical delocalization, thereby limiting attack by reactive species. Computational studies showed that these substitutions reduced spin density at the targeted sites. After synthesis of the four BDPA derivatives and radical generation, degradation rates were measured using both UV-vis and EPR spectroscopy. These studies confirmed that the most highly substituted derivative exhibited greater stability than unmodified BDPA under identical conditions. These functionalized BDPA radicals provide new experimental opportunities for developing more persistent carbon-based radicals for future DNP applications.

Olivia Woodward - Utah State University
0900 Old Main Hill Logan, Utah, 84322 United States, Email: olivia.woodward@gmail.com

Probing Cu^{2+} Dopant Sites in Zn-based MOF-74 via EPR Spectroscopy

Pranjit Das[1], Andreas Pöppl[1*]

[1]Felix-Bloch-Institute of Solid-State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, Linnéstrasse 5, Leipzig 04103, Germany

Metal-organic frameworks (MOFs) continue to attract significant attention due to their tunable pore structures, chemical versatility, and potential applications in gas storage, catalysis, and separations [1–4]. Among these, MOF-74 (also known as CPO-27) is a widely studied framework for the study of dihydrogen isotope separation and storage because of the presence of open metal sites [5,6]. Introducing paramagnetic dopants like Cu^{2+} in MOF74 (Zn) facilitates the utilization of electron paramagnetic resonance spectroscopy (EPR), which is very sensitive to the local environment of the probe.

We investigated Cu^{2+}-doped MOF74 (Zn), using EPR to study the structural properties of the framework for utilization in the field of dihydrogen isotope storage and separation. Upon measuring with continuous wave EPR, it is evident from the EPR parameters that the Cu^{2+} species are incorporated in a distorted octahedral environment. Treating the as-synthesized sample with pulsed EPR techniques like 2pESEEM, 3pESEEM, and HYSCORE spectroscopy reveals further details about how the Cu^{2+} species is incorporated into the framework. It is evident that the Cu^{2+} species is incorporated at a Zn^{2+} framework site and binding to five oxygens from the framework and one solvent molecule. Upon activation, the solvent molecule gets removed, and the local environment of the Cu^{2+} species changes. The formation of such an open metal site is crucial for future dihydrogen separation and storage applications of this material. Further EPR will reveal the host-guest interaction of the framework and the hydrogen gas molecules.

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Pranjit Das - Leipzig University
Linnéstraße 5 Leipzig, Saxony, 04103 Germany, Email: pranjit.das@uni-leipzig.de

The SMART Center: EPR Spectroscopy as a Teaching and Research Platform for the Broader Magnetic Resonance Community

Reef (Philip D., II) Morse

Steppingstone MAgnetic Resonance Training (SMART) Center, 650 Church Street Suite 110A, Plymouth, MI 48170

The Steppingstone MAgnetic Resonance Training Center[1,2,3] (SMART Center, Plymouth, MI) is designed to serve both as a hands-on research training environment for middle and high school students and as an open-access EPR facility welcoming academic and industrial researchers. Teaching: SMART Center students operate JEOL TE100 and RE1X, Bruker ESP300, Escan, and Micro spectrometers to pursue original research projects (examples are companion posters by Emily Cheng: “Measurement of TEMPO Reduction to Determine Storage Effects on Antioxidant Levels in Fruits and Vegetables III” and Amarachi Emole: “Can Metabolism Match Supplements? A Comparison of Antioxidant Effects on Free Radical Scavenging”). Software: Development of data acquisition (ew_daq, a Python-based replacement for legacy CW-EPR acquisition software supporting multiple spectrometer platforms), data analysis (ew_analyze, a node-based dataflow pipeline for automated spectral processing), and AI-assisted spectral analysis (NitroxideNet, a convolutional neural network trained on EasySpin-simulated nitroxide spectra that predicts X band Lorentzian and Gaussian linewidths with 5–7% median error ($4x10^6$-spectra training set). Instrumentation: A custom stop-flow/continuous-flow mixing apparatus enabling real-time kinetic EPR measurements with sub-second time resolution will be available for demonstration at the poster. Supported by Steppingstone School for Gifted Education, Bruker BioSpin, and Rotunda Scientific Technologies. The author thanks Boris Epel (University of Chicago) for EasySpin simulation support.

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Reef (Philip D., II) Morse - Steppingstone MAgnetic Resonance Training Center
650 Church Street, Suite 110A Plymouth, MI, 48170 United States, Email: reef@steppingstoneschool.org

Small Changes in Stereochemistry, Large Effects on Membrane Organization: An EPR Study of Glucosylceramides

Shayak Biswas,[1] Rajendra Rohokale,[1] Sayan Kundu,[1] Mingwei Zhou,[1] Md. Shamiul Islam,[1] Jiatong Guo,[1] Rajendra Mane,[1] Selena Dessain,[1] Gail E. Fanucci,[1] and Zhongwu Guo[1,2]

1. Department of Chemistry, University of Florida, Gainesville, Florida 32611, United States
2. UF Health Cancer Center, University of Florida, Gainesville, Florida 32611, United States

Glucosylceramides (GlcCers) are glycosphingolipids that play an important role in modulating membrane organization through interactions between their carbohydrate headgroups and surrounding lipid environments. Subtle differences in glycosidic stereochemistry can therefore have significant effects on their membrane behavior.

To investigate the effect of glycosidic bond stereochemistry on membrane behavior, a- and ß-anomeric glucosylceramides spin-labeled at the 6-position of the glucose moiety were incorporated into model lipid membranes and characterized using continuous-wave electron paramagnetic resonance (CW-EPR) spectroscopy and dynamic light scattering (DLS).

EPR spectroscopy was used to probe the local environment and rotational dynamics of the spin-labeled glycolipids within lipid bilayers. Distinct spectral differences were observed between the a- and ß-anomers, indicating differences in motional freedom, lipid packing, and membrane incorporation despite the two molecules differing only in the orientation of the glycosidic linkage. Analysis of the EPR lineshapes revealed that anomeric configuration significantly influences the organization of glucosylceramides within the membrane. DLS measurements complemented the EPR results by characterizing the size and stability of the lipid assemblies.

These findings demonstrate that subtle changes in carbohydrate stereochemistry can produce measurable effects on membrane structure and dynamics, and highlight the utility of spin-label EPR spectroscopy for investigating glycosphingolipid–membrane interactions.

Shayak Biswas - University of Florida
3800 SW 34th Street, O-120 Gainesville, Florida, 32608 United States, Email: biswas.shayak@ufl.edu

Atomistic pictures of slow protein conformational changes using EPR and simulations.

Shramana Palit, Darian T. Yang, Xiaowei Bogetti, Anthony Bogetti, Olivia Wood, Lillian T. Chong*, and Sunil Saxena*.

Department of Chemistry, University of Pittsburgh, Pittsburgh PA 15260, USA

Large-amplitude protein conformational changes are central to many cellular processes. However, capturing the pathways of these changes remains an extant challenge. Electron paramagnetic resonance (EPR) spectroscopy can report on these changes through distance measurements between site-directed spin labels, but does not provide atomistic resolution. Conversely, conventional molecular dynamics (MD) simulations offer detailed structural insight but often fail to access the long timescales over which such transitions occur.
In this work, we integrate weighted ensemble (WE) path sampling with EPR-measured distance restraints to directly capture the transition pathways between conformational states of lysine/arginine/ornithine binding protein (LAOBP). Using this approach, we generated hundreds of trajectories that describe the large-scale transition between the closed (ligand-bound) and open (ligand-free) states. Analysis of these pathways revealed key residue-level interactions that govern the transition. Guided by these insights, we performed selected mutagenesis that stabilized the protein in its open state. Together, these combined techniques allow the visualization of hidden alternate states while also providing a mechanistic understanding that guides the rational tuning of protein function.

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Shramana Palit - University of Pittsburgh
219 Parkman Ave Pittsburgh, PA, 15260 United States, Email: shp176@pitt.edu

Decoherence of Nitroxide Spin Labels On Proteins

Samuel M. Jahn, Afrah Aftab, Rachelle K. Stowell, Maxx Tessmer, Stefan Stoll

Department of Chemistry, University of Washington, Seattle, WA, USA

Spin-labeling of proteins with nitroxide radicals is valuable both for characterizing protein conformational landscapes by EPR spectroscopy and for providing structurally precise scaffolds for potential spin qubit-based quantum sensing applications. At cryogenic temperatures, the phase memory times of nitroxide radicals, critical to both applications, are governed by the density and spatial distribution of nuclear spins, principally protons, within the unpaired electron's nanoenvironment. We employ an integrated computational approach combining protein structural modeling with spin dynamics simulations to predict nitroxide Hahn echo decoherence dynamics as a function of labeling site, with predictions that compare favorably against experimental data for maltose-binding protein. The spin dynamics simulations invoke an extended cluster correlation expansion (CCE) formalism that explicitly accounts for dynamic state-mixing effects arising from tunneling methyl groups on amino acid side chains. Finally, we demonstrate that phase memory times can be predicted semi-quantitatively from the structure of the spin-labeled protein alone without recourse to full quantum simulations via a simple empirical relation parameterized by local proton and methyl group counts.

Stefan Stoll - University of Washington
Box 351700 Seattle, WA, 98195 United States, Email: stst@uw.edu

Electrostatic Environment in Phospholipid Vesicles: Layer by Layer, Inside and Out

Ngan Nguyen, Maxim A. Voinov, Alex I. Smirnov, Tatyana I. Smirnova

North Carolina State University, Raleigh, NC

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. One method for assessing surface electrostatics involves determining the pK_a shift of protonatable molecular probes. Previously, we successfully employed EPR of phospholipids labeled at the headgroup with a pH-sensitive nitroxide to map bilayer interfacial electrostatics. Here, we report on a comparative study of the surface electrostatics of multilamellar (MLVs) and unilamellar vesicles (ULVs) composed of either POPG or POPC lipids. For vesicles composed of negatively charged POPG, the effective pK_a measured for MLVs was significantly, up to 0.9 pH unit, higher than that for ULVs across all three probes. The larger local electrostatic potential experienced by probes within the inner lamellae is likely due to an influence of charges on the adjacent lamellae. For zwitterionic POPC, the effective pK_a for MLVs was only slightly lower than that for ULVs, suggesting that the electrostatic environment in the inner lamellae closely resembles that of the outermost and innermost layers, with minor differences potentially arising from variations in hydration and ion distribution. We then measured the protonation state of probes at the surfaces of outer or inner leaflets of DMPG ULVs and observed a significant shift in pKa, indicating a difference in electrostatic or local dielectric environments of the probes. The results further highlight the utility of the spin-labeled phospholipids in biophysical EPR spectroscopy and reveal unexpectedly large changes in layer-dependent electrostatic environments in MLVs and ULVs. This material is based upon work supported by the National Science Foundation under Grant No. 2305172

Tatyana Smirnova - North Carolina State University
2620 Yarbrough Dr, NCSU Raleigh, NC, 27695 United States, Email: tismirno@ncsu.edu

Direct Detection of Multiple Distance Peaks from Pulsed Dipolar Signal

Utkarsh Misra[1,3], Shikhar Prakash[1], Aritro Sinha Roy[2,3], Jack H Freed[2,3], Madhur Srivastava[2,3,4,*]

[1] Department of Systems Engineering, Cornell University, Ithaca, NY 14850, United States
[2] Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, 14850, United States.
[3] National Biomedical Resource for Advanced ESR Spectroscopy, Cornell University, Ithaca, NY 14853 USA.
[4] Cornell Atkinson Center for Sustainability, Cornell University.

Here, we introduce an independent comparison framework for pulsed dipolar electron spin resonance. Recovering distance distributions P(r) from PDS time-domain signals is an ill-posed inverse problem, and samples with different underlying distance distributions can sometimes produce nearly indistinguishable time-domain signals, making it useful to have an additional way to confirm whether two samples truly differ in conformation. The framework quantifies differences in the underlying distance distributions directly from PDS signals, without relying solely on full distribution reconstruction.
The resulting dissimilarity metric offers several advantages: (1) it reliably determines the number of peaks present in a distribution; (2) it distinguishes two closely spaced peaks from a single broader peak once their separation exceeds 1 Å; (3) it recovers peak positions and mixture compositions in overlapping distributions and (4) it correlates systematically with differences in the distance distributions. All while remaining consistent with results from established reconstruction methods.
The framework leverages a time-frequency domain representation of PDS signals to enable this direct, quantitative comparison. Signals are transformed using continuous wavelet transforms and compared using the structural similarity index measure (SSIM). We validate this approach on simulated distance distributions as well as experimental data from rigid biradicals and SOD1 mutants linked to amyotrophic lateral sclerosis (ALS), where the results closely match those obtained from established methods.
This time-frequency comparison framework offers a complementary, reconstruction-independent strategy for confirming differences in distance distributions between PDS samples, with particular value for distinguishing closely related or highly overlapping conformational states in proteins.

Utkarsh Misra - Cornell University
116, Thurston Avenue Ithaca, New York, 14850 United States, Email: um48@cornell.edu

Organic Radical Dendrimers as Metal-Free T1 MRI Contrast Agents

Vega Lloveras,[1,2] Yufei Wu,[1] Chuanting Zhou,[1] Ehsan Shirdel,[1] Xuejiao Wang,[1] Songbai Zhang,[1] Luiz Pinto,[1] and José Vidal-Gancedo.[1,2]

1. Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), carrer dels Til.lers, 08193 Cerdanyola del Vallès, Spain
2. CIBER de Bioingeniería, Biomateriales y Nanomedicina, CIBER-BBN, 08913 Cerdanyola del Vallès, Spain.

Early detection of tumors is essential for improving patient survival, making magnetic resonance imaging (MRI) one of the most valuable tools for cancer diagnosis and monitoring. Although gadolinium-based contrast agents (GBCAs) remain the clinical standard for T1-weighted MRI, concerns regarding their toxicity have driven the development of safer, metal-free alternatives.
Persistent organic radicals are promising T1 contrast agents, but their clinical translation is hindered by low relaxivity and rapid bioreduction under physiological conditions. These limitations can be overcome by grafting multiple nitroxide radicals onto dendritic macromolecules, which enhance both relaxivity and radical stability through multivalency and steric shielding. Unlike conventional polymers, dendrimers offer well-defined architectures that enable precise control over radical number and spatial distribution.
Here, we report the synthesis of several generations of water-soluble radical dendrimers fully functionalized with peripheral nitroxide radicals.[1–4] Water solubility was achieved using either amino acid or PEG linkers, with amino acid-based dendrimers exhibiting superior performance.[4] EPR spectroscopy combined with molecular dynamics simulations revealed that radical location, water accessibility, and hydrogen-bonding interactions with nitroxide groups are key determinants of relaxivity.[3,4]
In vitro and *in vivo* MRI studies demonstrated that higher-generation radical dendrimers provide contrast enhancement comparable to, or greater than, commercial GBCAs.[1–4] In a murine GL261 glioblastoma model, they selectively accumulated in tumor tissue, enabling prolonged imaging (>2.5 h), while exhibiting high biological stability and renal clearance. These results highlight their potential as metal-free MRI contrast agents.

1. Pinto et al., *ACS Appl. Bio Mater.,* 2020, *3*, 369.
2. Zhang et al., *Biomacromolecules* 2022, *23*, 2767.
3. Wu et al., *Acta Biomater.* 2025, *192*, 461.
4. Wu et al., *ACS Polym. Au*, 2026, *6*, 3, 806.

José Vidal-Gancedo - Institut de Ciència de Materials de Barcelona (ICMAB–CSIC)
Carrer dels Til.lers, 08193 Cerdanyola del Vallès, Spain Cerdanyola del Vallès, Barcelona, 08193 Spain

Silicon L-Center Characterization via Orientation-Selective High-Field EPR

Wei-Hsu Lin,[1,2] Alex Giovannone,[1,2] Cody Fan,[3] Robert Krumland-Dunning,[1,2] Juan Felipe Gaitan,[1,2] Nikolay I Agladze,[1,2] Avik Pamarthi,[3] Murat Can Sarihan,[3] Jin Ho Kang,[3] Chee Wei Wong,[3] Mark S. Sherwin[1,2]

Department of Physics, University of California, Santa Barbara, California 93106, USAInstitute for Terahertz Science and Technology, University of California, Santa Barbara, California 93106, USADepartment of Electrical and Computer Engineering, University of California, Los Angeles, California 90095, USA

We present the application of a software-controlled two-axis rotating sample holder for high-field, orientation-selective (rotating) electron paramagnetic resonance (EPR) studies of the silicon L-center, an underexplored color center of interest for quantum information technologies. Silicon color centers are promising candidates for scalable quantum devices because they are compatible with existing CMOS fabrication processes and exhibit telecom-band optical emission, enabling scalable integration with both photonic and semiconductor platforms. While the optical properties and basic EPR response of the L-center have recently been characterized through a collaboration between the Sherwin Group and the UCLA Wong Group, its structure and symmetry remain poorly understood, motivating orientation-selective EPR measurements.

The Sherwin Group has developed a custom rotating sample holder for use in various cryogenic, high-?eld EPR experiments. Constructed entirely from EPR-silent materials and driven by a piezoelectric motor (attocube ANR51/RES/LT/HV), it is capable of operating at temperatures down to 1.6 K and magnetic fields up to 16 T. The adoption of a piezoelectric motor instead of conventional gear mechanisms greatly reduces design complexity and kickback, enabling an angular precision of ˜0.05° at room temperature and ˜0.1° under cryogenic, high ?eld settings with high reproducibility.

Using this instrument, we performed out-of-plane rotating EPR measurements at 80 K on the dominant resonance peak of the L-center (g ˜ 2.0007). Within our experimental uncertainty, no measurable angular dependence was observed, indicating that this axis is effectively isotropic. This result places new constraints on the symmetry of the proposed structure of the L-center, while comprehensive three-axis orientation studies are currently underway.

Wei-Hsu Lin - UC Santa Barbara
Department of Physics Broida Hall, University of California Santa Barbara Santa Barbara, California, 93106 United States, Email: wei-hsu@ucsb.edu

Photoexcited transient EPR of tetrakis(4-carboxyphenyl)porphyrin (TCPP), with differing ions, as ligands in zirconium MOFs towards quantum sensors and DNP transfer

Wern Ng[1], Jacob M. Lessard[2], Prathami Divakar Kamath[3], Chongwei Zhang[1], Jessica Yujie Wu[1], Ah-Young Song[1], Emanuel Druga[1], Kyriakos C. Stylianou[2], Jeffrey A. Reimer[1], Ashok Ajoy[1]

1. Department of Chemistry, University of California, Berkeley, CA, USA
2. Materials Discovery Laboratory (MaD Lab), Department of Chemistry, Oregon State University, Corvallis, OR, USA
3. Department of Materials Science and Engineering, University of California, Berkeley, CA, USA

Molecules with strong electron spin polarization have been used as quantum sensors and for enhancing nuclear spins through dynamic nuclear polarization (DNP)[1,2]. However, despite strides in transferring such polarization to more common chemical systems, the overall enhancement factors can still be improved. We here analyze the triplet electron spin dynamics of tetrakis(4-carboxyphenyl) porphyrin (TCPP) linkers within the zirconium based MOF-525 at room temperature and cryogenic temperatures using a homebuilt electron paramagnetic resonance (EPR) spectrometer at X-band. The transient EPR signals are detected from the porphyrin triplet states after pulsed laser excitation at 527 nm. We will present the effects of differing metal ions within the porphyrin linkers on the electron spin lattice relaxation times, alongside population analysis of the triplet sublevels. The incorporation of the triplet molecule as a linker within the MOF, coupled with the biocompatibility of MOF-porphyrins[3], strives towards realizing “bulk-as-sensing” platforms that may utilize DNP on adsorbed analytes for sensing. Longer relaxation times would be advantageous for bestowing the electron spin polarization to analytes adsorbed onto the MOF.
Mena et al., *Phys. Rev. Lett.* 2024, 133, 120801Singh et al., *Nat Commun* 2025, 16, 10530Chen et al., Angew. Chem. Int. Ed. 2021, 60, 5010.

Wern Ng - University of California Berkeley
University of California Berkeley, Tan Kah Kee Hall Berkeley, California, 94720 United States, Email: wern.ng@berkeley.edu

Robust AC Vector Sensing with Pentacene and Enhancing Spin Coherence by Nuclear Spin Hyperpolarization

Boning Li,1 Patrick Hautle,2 Duhan Zhang,3 Tom Wenckebach,2 Paola Cappellaro,1 and Yifan Quan3

1Department of Physics, Massachusetts Institute of Technology, MA 02139, USA
2PSI Center for Neutron and Muon Sciences, CH-5232 Villigen-PSI, Switzerland
3Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA

Molecular spin based quantum sensors offer a range of advantages, from high spin density to functionalization via chemical tunability. Here, we demonstrate microwave vector magnetometry using the photoexcited spin triplet of deuterated pentacene molecules, operating at zero external magnetic field and room temperature. We achieve full three-dimensional microwave field reconstruction by detecting the Rabi frequencies of anisotropic spin-triplet transitions associated with two crystallographic orientations of pentacene in naphthalene crystals [1]. We further introduce a phase alternated protocol that extends the rotating-frame coherence time by an order of magnitude. These results establish pentacene-based molecular spins as a practical and high-performance platform for microwave quantum sensing, and the control techniques are broadly applicable to other molecular and solid-state spin systems.

We furhter demonstrate a sizable increase in the coherence time of a pentacene electronic spins by hyperpolarizing the proton spin bath. We leverage the high electron spin polarization of pentacene generated via optical excitation, enabling high nuclear spin bath polarization (> 60%) via dynamic nuclear polarization. The polarized nuclear spin bath provides a reduced magnetic noise environment, leading to enhanced electron spin coherence even under repeated triplet-state excitations [2]. These observations are supported by a theoretical model and cluster correlation expansion (CCE) simulations. Together, these results establish nuclear spin hyperpolarization as a practical and controllable route to engineering photo-addressable molecular qubit platforms.

Yifan Quan - University of Pennsylvania
231 S. 34 Street Philadelphia, PA, 19104 United States, Email: yquan@sas.upenn.edu

EPR Characterization of Redox- and Topology-Dependent Spin Coupling in Diboron-Incorporated Indenofluorenes

Yujie Zhao, Bi Youan E Tra, Colleen H. McAloon, Andrew Molino, Chunlin Deng, Yifu Ouyang, Peter Mullër, David Wilson, Robert Griffin, Robert Gilliard

Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139, USA

Boron-doped polycyclic p-systems provide a flexible platform for tuning open-shell electronic structure, but assigning the spin state requires direct magnetic resonance characterization. Here, continuous-wave and pulsed EPR spectroscopy are used to examine spin coupling and spin delocalization in diboron-incorporated indenofluorene radicals and diradicals. In ligand-stabilized diboraindeno[1,2-b]fluorenes, chemical reduction gives open-shell singlet diradicals with thermally accessible triplet states. X-band CW EPR and Q-band echo-detected field-sweep measurements show triplet features together with an S = 1/2 monoradical impurity contribution. Microwave power-dependent CW EPR and nutation experiments were used to resolve the triplet signal and support the S = 1 assignment. In a second family of aryl-substituted diboron indenofluorene isomers, removing strongly p-accepting carbene ligands shifts the electronic structure toward the conjugated molecular core. The EPR-active meta-quinodimethane-like DB[2,1-b]IF reduced species include a 19p radical anion and 20p triplet diradicals. The radical anion shows boron and proton hyperfine couplings consistent with spin delocalization across the p-framework, while the triplet diradicals display small zero-field splitting parameters, indicating weak dipolar coupling between delocalized spins. In contrast, the para-quinodimethane-like DB[1,2-b]IF dianion favors a closed-shell singlet structure and serves as a useful comparison. Together, these studies show how EPR distinguishes radical impurities, doublet radicals, triplet diradicals, singlet–triplet energetics, and ligand-versus-core spin delocalization in main-group open-shell molecules.

Yujie Zhao - Massachusetts Institute of Technology
170 Albany Street, NW14 Francis Bitter Laboratory Boston, MA, 02139 United States, Email: yujiez@mit.edu

Next-Generation EPR: Combining High-Performance Q Band Instrumentation with Artificial Intelligence Enhanced Spectral Processing

Yang Zhou, Zhuoyang Qin, Yue Zhang, Zhiyu Jeff Sun, Zhifu Richard Shi, Kebiao Xu

CIQTEK Co., Ltd., No. 1969, Kongquetai Road, HeFei High Tech Zone, AnHui, China

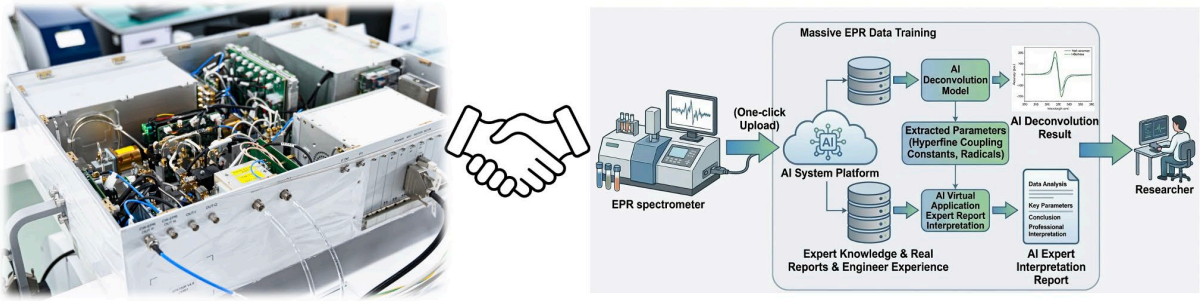
Keywords: Q Band EPR, AI Spectral processing, Automatic Report Generation, Solid-State Power Amplifier

The advancement of Electron Paramagnetic Resonance spectroscopy is increasingly defined by the convergence of robust hardware and intelligent software. While EPR remains a vital tool for probing paramagnetic centers, broader adoption is limited by instrument complexity and the steep learning curve of spectral analysis. Researchers at CIQTEK address these barriers by developing high-performance hardware alongside the first dedicated AI model for EPR.

Our Q-band pulsed EPR system achieves less than 10 ns π/2 pulse wide-bandwidth excitation using a Solid-State Power Amplifier, offering superior longevity and reduced maintenance over conventional technology. This architecture maximizes sensitivity and spectral resolution, deciphering complex metal hyperfine couplings and extracting dipolar information for high-resolution DEER distance mapping.

Complementing the hardware is a three-layer AI EPR model that streamlines the workflow from raw data to publication. Trained on over 100,000 real and simulated datasets — achieving 99.9% precision for simulations and 92% for real-world samples — the model automates spectral fitting, component characterization, and experimental report generation. It further offers predictive guidance, suggesting follow-up experiments to validate findings.

This integrated approach lowers the entry barrier for researchers in chemistry, biology, and materials science, driving EPR toward a more impactful technology.



Zhiyu Sun - CIQTEK
No. 1969, Kongquetai Road, High-tech Zone Hefei, Anhui, 230088 China, Email: xiaxy@ciqtek.com

Very High Frequency (263 GHz) Pulse EPR Spectroscopy of High Spin Transition Metal Centers

Zikri Hasanbasri[1], Shasha Qiu[2], Guodong Rao[1], Amanda Caceres[1], Erica Debley[3], Pan Pan[4], Yuan Zheng[5], Ying Li[4], Jinjun Feng[4], Elizabeth M. Nolan[3], Marie Heffern[1], Paul Stucky[1], Neville C. Luhmann, Jr.[2], R. David Britt[1]

Department of Chemistry, University of California Davis, 1 Shields Ave, Davis, CA, 95616, USA. Department of Electrical and Computer Engineering, University of California Davis, 1 Shields Ave, Davis, CA, 95616, USA. Department of Chemistry, Massachusetts Institute of Technology, Cambridge MA, 02139, USA. National Key Laboratory of Science and Technology on Vacuum Electronics (NKLST-VE), Beijing Vacuum Electronics Research Institute (BVERI), Beijing, 100015,China. National Key Laboratory of Science and Technology on Vacuum Electronics (NKLST-VE), University of Electronic Science and Technology of China (UESTC), Chengdu, China.

Pulse Electron Paramagnetic Resonance (EPR) spectroscopy provides powerful tools for examining species with unpaired electrons, such as organic radicals and metal ions, in a wide variety of interesting systems. However, the lack of high-power pulse amplifiers at frequencies above 95 GHz has restricted their application at very high frequencies. Here, we showcase the development of a 10 W traveling-wave vacuum tube amplifier at 263 GHz, employed in a pulse EPR spectrometer. Pulse EPR at this high frequency is particularly useful for studying transition metals with S>1/2 that have large, broadening effects from "zero-field splitting" interactions, which often dominate the EPR spectra obtained at low frequencies. We show that the pulse EPR spectrometer at 263 GHz has a superb limit of detection, capable of resolving transition-metal impurities in a diamagnetic material. Furthermore, we highlight the resolution of the EPR spectra from a series of high-spin (S=5/2) Mn(II) complexes with metal sequestering proteins, in which the ZFS and the individual transitions are visibly differentiated.
Supported by NIH MIRA (R35GM126961) and DOE (DE-SC0025948 and DE-SC0007203).

Zikri Hasanbasri - University of California - Davis
141 Physical Sciences Mall, Chemistry Loading Dock Davis, California, 95616 United States, Email: zhasanbasri@ucdavis.edu

ACERT: A Service Resource for ESR Researchers

Madhur Srivastava

Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY 14853, USA National Biomedical Resource for Advanced ESR Spectroscopy, Cornell University, Ithaca, NY 14853 USA

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. We plan a regular series of workshops to be devoted to training students and researchers in the latest technologies.

Madhur Srivastava - Cornell University
155 Baker Lab Ithaca, New York, 14853 United States, Email: ms2736@cornell.edu

301 **SSNMR Oral Session**

MAS meets order – from oriented micro-crystals to secular dipolar order –

Kazuyuki Takeda

Kyoto University, Division of Chemistry, Graduate School of Science, 606-8502 Kyoto, Japan

We roll out our recent fresh pairings of hitherto unlinked subjects, including (i) MAS and secular dipolar order[1], (ii) MAS and oriented micro-crystals, (iii) Triplet DNP and overtone polarization[2], and (iv) metal-organic framework (MOF) and para-hydrogen generation[3]. To summarize each topic's takeaway, dipolar order can develop in first order under MAS, if it is created in the nutating frame of reference[1]. MAS of Magnetically Oriented Microcrystal Array (MOMA) mimicking MAS of a single crystal brings about an effective way toward determining the orientation of chemical shift tensors even when a large enough crystal is hard to grow. The overtone transition of electron spins in the photo-excited triplet state can draw nearly full participation of electron spin packets to polarization transfer in powder where the anisotropy of the zero-field splitting interaction severely broadens the electron's resonance and limits tapping of the polarization resource if one resorts to the conventional single-quantum transition[2]. Undiluted and activated Ni-MOF-74 is a stunningly efficient converter of nuclear-spin isomers of molecular hydrogen compared to a published reports of alumina-diluted Ni-MOF-74, and paves the way for ultra-efficient para-hydrogen generation[3].
[1] K. Suzuki, and K. Takeda, Phys. Rev. Lett. 135, 188001 (2025).
[2] K. Miyanishi, T.F. Segawa, M. Negoro, A. Kagawa, and K. Takeda, Phys. Rev. B 113, 024311 (2026).
[3] Y. Noda, K. Fuchibe, M. Mukoyoshi, and K. Takeda, chemrxiv.15000923.

Kazuyuki Takeda - Kyoto University
Rm 377, Building 6, Kitashirakawa-Oiwakecho, Sakyo Kyoto, Kyoto, 606-8502 Japan, Email: takezo@kuchem.kyoto-u.ac.jp

Design of a Triple-Resonance (1H/13C/17O), Cryogenic, DNP-MAS Transmission Line Probe for an 800MHz Spectrometer

Nicholas Wiesner*, Samuel Strymish*, Daniel Banks, Natalie Golota, Ravi Shankar Palani, Lauren Shaffer, Robert G. Griffin

*Authors contributed equally to this work

Massachusetts Institute of Technology, Department of Chemistry, Cambridge, MA 02139

We report the design and construction of a triple-resonance ($^{1}H/^{13}C/^{17}O$), cryogenic, modular, dynamic nuclear polarization (DNP) compatible, magic angle spinning (MAS) probe, based on transmission line components and its implementation in an 800MHz spectrometer with a 527GHz solid state microwave source. The probe utilizes stepped transmission lines and remote tuning to achieve exceptionally high Rabi frequencies for the sample size of 1.3mm (up to 270kHz ^{1}H) as well as isolation of =18dB between all channels. Higher Rabi fields are important to avoid finite pulse effects especially with high spinning frequencies. Also, higher ^{1}H Rabi fields improve ^{1}H decoupling, decreasing linewidths. We achieved a DNP enhancement of up to ~70 on ^{13}C nuclei in a P1 diamond sample with only 30mW of microwave power (see Figure 1). Circuit topology is displayed on the right side of Figure 2. First, the complex sample chamber is constructed and characterized. Next, required input impedances are calculated such that a current maximum is created at the center of the coil, indicated by a black dot. Two other current maxima, also indicated by black dots, provide inter-channel-isolation at junction points. To transform impedances between the nodes and the sample chamber, two stepped transmission lines were designed. A stepped transmission line is one whose dielectric and cross-section change along its length. We wrote a gradient descent program to optimize these lines that takes loss into account.

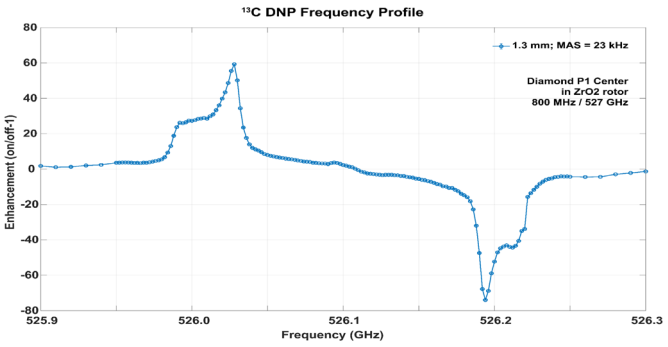


Figure 1. ^{13}C Zeeman field profile obtained from a P1 diamond sample. Shown is the DNP enhancement vs. frequency using an AWG to sweep from 529.9→526.3 GHz. T=298 K, $w_r/2p$=23kHz.

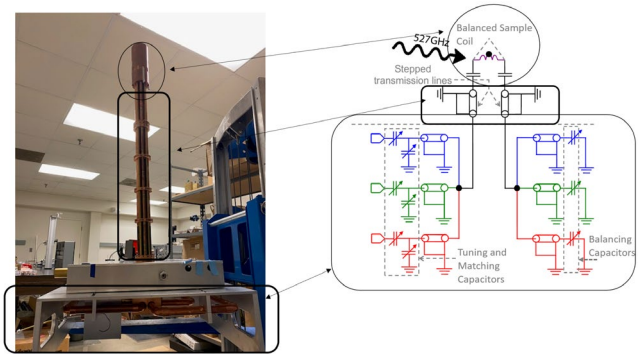


Figure 2. The assembled probe corresponding circuit diagram. The relationship is indicated with boxes and arrows. (circuit diagram adapted from [1])

Samuel Strymish - Massachusetts Institute of Technology
77 Massachusetts Avenue, Cambridge, MA 02139, USA Cambridge, MA, 02139 United States, Email: sstrymis@mit.edu

Advances in Sensitivity and Photoillumination Technology for Magic-Angle Spinning Probes

Lauren E. Price[1], Charles G. Mullen[2], Alex S. Drena[1], Mario Incitti[2], Benjamin D. Harding[1], Jesse Ransom[1], John A. Stringer[2], Chad M. Rienstra[1]

1 Resynant, Inc., 2001 Terrace Avenue, Suite 203C, Middleton WI 53562
2 PhoenixNMR, 510 E. 5th Street, Loveland CO 80573

Recent advances in probe technology have substantially improved the sensitivity and experimental scope of solid-state NMR under MAS conditions. These developments enhance existing standard experiments while also enabling novel experiments. One such advance is a crossed coil probe design that doubles the sensitivity for ^{1}H-detected SSNMR. A second major advance is photoillumination during MAS. This technology enables a range of applications including CIDNP experiments, in situ pH measurements, and the study of light induced structural changes. We describe such a probe that allows for both radial and axial irradiation of the sample, achieving several-fold improvements in photoconversion of standard azobenzene dyes. Fiber optic and mirror placement enables both modes of illumination without any compromise in probe efficiency, lineshape, spinning or temperature range. Multiple wavelengths of light can be utilized for reversible photoconversion and time synchronization of the light with NMR pulse sequences. We anticipate a range of high impact applications of this technology for the SSNMR community.

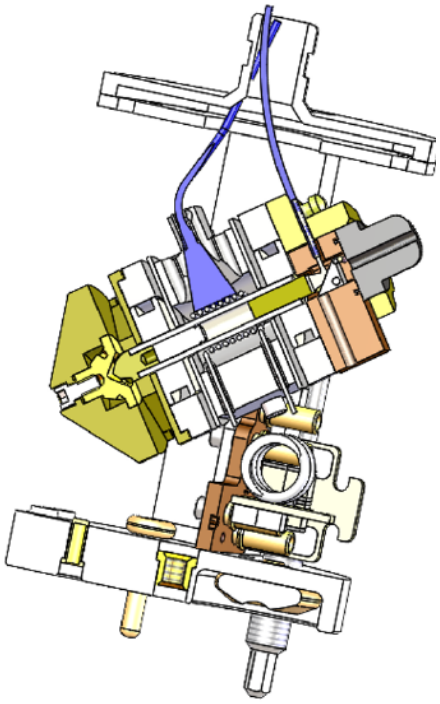


Figure 1 CAD (computer assisted drawing) of the photo illumination probe head. Illumination of the sample can be either axial or radial.

Lauren Price – Resynant
8001 Terrace Avenue, Suite 203C Middleton, Wisconsin, 53562 United States, Email: lauren@resynant.com

Rethinking MAS NMR with Additive Manufacturing: Optimized 3D-Printed RF Coils and Single-Sided MAS of Planar Samples

Thomas Osborn Popp,[1] Konstantin Drallios,[1] Gemma Pham,[1] Ryan Galperin[1], Andrew Dufur,[1] Aidan Cuccaro,[1] Mithun Karthikeyan[1]

1. Oregon State University, Department of Chemistry, Corvallis, OR, 97331

Here we present our latest efforts to use additive manufacturing to develop MAS NMR hardware that is no longer limited to fixed conventional geometries, but can instead be customized for performance, have easily replaceable components, and be adapted to new classes of samples. We demonstrate metallized 3D-printed RF coils, in which stereolithographically printed structures are converted into functional copper conductors by electroless deposition and electroplating.[1] In combination with CAD-based Biot-Savart field calculations, this workflow enables the direct fabrication and testing of sample-volume-optimized coil geometries. As a representative example, a tilted-helix variable-pitch solenoid yields a 22% higher B_1 field and an 11% longer homogeneous region compared to a standard solenoid. We also present a fully replaceable 3D-printed stator for standard 5 mm cylindrical rotors designed for use in commercial probes, reducing the consequences of rotor crashes while supporting training, prototyping, and exploratory measurements. Finally, we describe our development of single-sided MAS for surface-sensitive NMR of planar samples, in which flat samples are spun at the magic angle and detected by a surface coil placed in close proximity to the sample face. This geometry extends MAS NMR to films, coatings, substrates, and other planar samples poorly served by cylindrical rotors. Together, these developments establish 3D printing as a functional platform for MAS NMR hardware that is not only more accessible and repairable, but also recaptures some of the instrument-building flexibility that helped to define early MAS NMR, enabling components to be optimized for specific experimental goals.

1. Drallios et al., 2026. Metallized, 3D-printed radiofrequency coils. *J. Magn. Res.*, 108057.

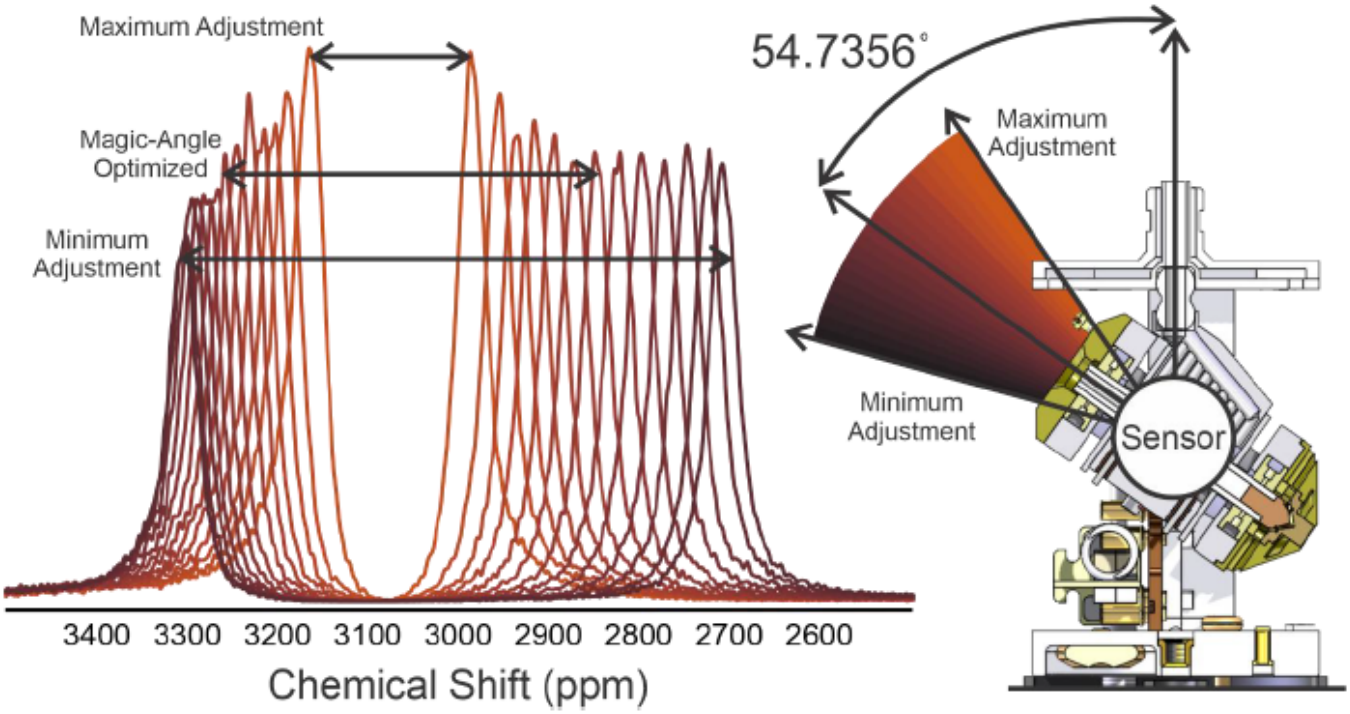
Thomas Osborn Popp - Oregon State University
153 Gilbert Hall Corvallis, OR, 97330 United States, Email: osbornpt@oregonstate.edu

Setting the Magic-Angle with a Probe-Integrated Independent NMR-Based Sensor

Marcus D. Tuttle,[1] John A. Stringer[1]

PhoenixNMR LLC, Loveland CO 80534

Accurate and precise optimization of the magic-angle (MA) is crucial for the success of MAS ssNMR experiments. How well the MA is set influences both the resolution of the spectrum as well as the efficiency of recoupling elements in the pulse sequences. Offsets as small as 10-20 millidegrees can lead to measurable broadening of signals, and for the most demanding experiments, such as ST-MAS, the angle must be set within 1-2 millidegrees of the MA. Despite the level of precision needed, a combination of the limited material choices available for probe building, mechanical stability of the MA, and optimization procedures (such as use of an external reference compound), can lead to MA offsets that can be unknown, ignored, and/or difficult to optimize. Here, we present a dedicated magic-angle sensor integrated into a PhoenixNMR MAS ssNMR probe head. This sensor utilizes a separate RF channel affixed to the MAS spinning module. The orientation of the sensor is calibrated such that when a rotor is aligned along the MA, the position of signals in the sensor are known. We show that the angle of the module can be set to any angle using spectra acquired by the sensor. This assembly allows for the adjustment of the magic angle at any time, with precision limited by the precision of the calibration, set during the initial installation of the probe head.



Marcus Tuttle - PhoenixNMR LLC
510 E 5th Street Loveland, CO, 80537 United States, Email: mt@phoenixnmr.com

Explorations of membrane-active peptide partitioning, lipid phases, and pH in pulmonary surfactant

Joanna R. Long, Mahsa Moshari, Ritu Kaushik, Shayak Biswas, Alexander Gannon, Logan Delgado, Gabrielle Salvadori, Katherine Gorkov, Diana Tymochko, Nhi, Tran, Lauren Schaffer, M. Luiza Caldas Nogueira, Faith Scott, Shuba Gunaga, Frederic Mentink-Vigier, and Gail Fanucci

University of Florid and U.S. National High Magnetic Field Laboratory

Membrane-active peptides derived from Surfactant Protein B (SP-B) exhibit unique abilities to modulate lipid phase properties. Using ssNMR, EPR, and MAS-DNP methodologies, we are mapping out the properties of model pulmonary surfactant (PS) formulations that mimic the native lung environment and therapeutic formulations used to treat acute respiratory distress in premature infants. By characterizing lipid phases and dynamics in concert with peptide structure, partitioning, and dynamics as a function of pH and temperature, we observe how differential partitioning of amphipathic PS peptides in response to environmental conditions leads to the unique lipid phase behaviours observed in PS. Our observations point to a novel mechanism for trafficking of dipalmitoylphosphatidylcholine (DPPC), the primary lipid in PS, to the air-water interface to lower surface tension and support breathing at ambient pressures. As part of my presentation I will highlight recent advances in MAS-DNP, rarely utilized ssNMR approaches for mapping out lipid dynamic, and complimentary EPR measurements that enabled us to develop a holistic understanding of the elegant molecular biophysics underlying PS function.

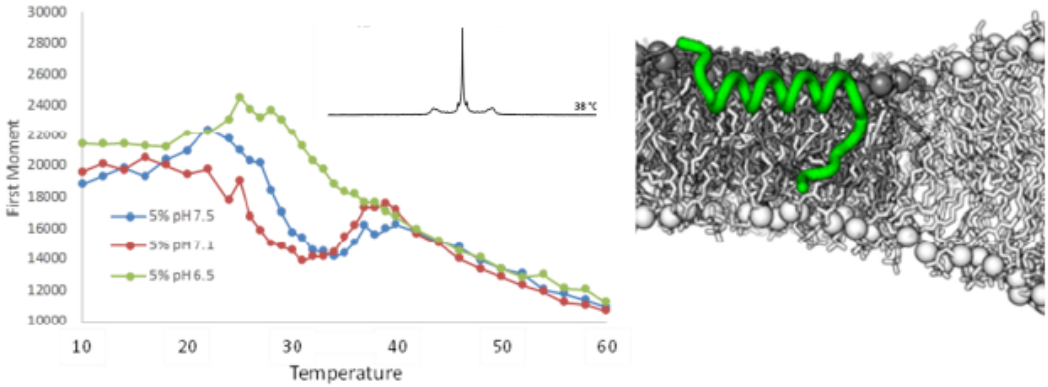


Figure 1. At physiologic temperature, the N-terminus of surfactant protein B induces cubic and interdigitated lipid phases as measured by ^{2}H NMR of lipid acyl chain dynamics. The balance of cubic and interdigitated phases are sensitive to small changes in environmental pH.

Joanna Long - University of Florida
PO Box 100245 Gainesville, FL, 32610 United States, Email: jrlong@ufl.edu

A Model for Solid-State NMR Studies of FG-Repeat Peptides under Nanopore Confinement

Wancheng Zhao, Wai-Ming Yau, and Robert Tycko

Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD 20892-0520

Intrinsically disordered phenylalanine-glycine (FG) repeat segments tethered to the inner surfaces of nuclear pore complexes are biologically important for selective nucleocytoplasmic transport. Disturbances in this FG-mediated selectivity are broadly implicated in cancer, neurodegeneration, and viral infection. However, the low sequence complexity, weak net charge, and aggregation tendency of FG repeats have impeded mechanistic insight into how their structure and dynamics underlie FG barrier function and disease relevance. In this study, we introduced an experimental approach for solid-state nuclear magnetic resonance (ssNMR) studies of FG-repeat sequences (or other polypeptides) covalently tethered to nanopore walls. Isotope-labeled FG30 peptide, a 30-residue segment from the FG-repeat domain of human Nup98 nucleoporin, was covalently tethered to anodic aluminum oxide (AAO) wafers with 20nm-nanopores via phosphonate surface chemistry. ^{13}C and ^{1}H NMR chemical shifts indicate that FG30 chains are dynamically disordered and random-coil-like in buffer-filled pores. Spin relaxation data for ^{13}C-labeled sites show smooth dependences of relaxation times on temperature, which rules out a temperature dependent phase transition. Quantitative ssNMR analysis indicated an exceptionally high FG30 peptide concentration (~ 300 mg/mL or 90 mM) in the confined AAO pores, yet no aggregation was detected over several months. In contrast, unbound FG30 at only 2 mM in the same buffer rapidly formed fibrillar aggregates within days. By contrast, replacing FG30 with melittin in the same hydrated AAO-nanopore tethering format led to a markedly different state: most melittin chains showed restricted motions and adopted a-helical conformations, instead of remaining highly dynamic as FG30. Thus, effects of tethering and nanopore confinement are clearly sequence-dependent for peptides of similar length. These findings suggest that nanoscale confinement and surface tethering may modulate the phase behavior of intrinsically disordered FG-repeat proteins. It also demonstrates the utility of AAO as a scaffold for studies of polypeptides in nanopore-confined environments and under disease-relevant perturbations.

Wancheng Zhao - National Institutes of Health
5 Memorial Drive, Building 5 Bethesda, MD, 20892 United States, Email: wancheng.zhao@nih.gov

An eye lens protein forms a transparent gel via nonspecific transient interactions

Jaewon Suk,[1] Ravi S. Palani,[2] Hao-Wei Shih,[3] Robert G. Griffin,[2] Jin K. Montclare,[3] and Rachel W. Martin[1,4].

1. University of California, Irvine, Department of Chemistry, Irvine, CA 92697
2. Massachusetts Institute of Technology, Department of Chemistry, Cambridge, MA 02139
3. NYU Tandon School of Engineering, Department of Chemical and Biomolecular Engineering, New York, NY 11201
4. University of California, Irvine, Department of Molecular Biology &; Biochemistry, Irvine, CA 92697

The eye lens is a transparent proteinaceous organ with hydrogel-like characteristics, where protein concentrations reach upwards of 400 mg mL^{-1}.[1,2] Within the lens proteome, crystallins participate in protein-protein interactions that facilitate lens health and its refractive properties.[2] In this study, we investigate how intermolecular interactions between monomeric human gS-crystallin facilitate lens protein phase transition. Using MAS ssNMR, ^{15}N-^{13}C ZF-TEDOR and ^{13}C-^{13}C RFDR spectra of gS-crystallin semi-solids show minimal backbone chemical shift perturbations that would be indicative of strong binding. ^{13}C-^{15}N Isotope mixing experiments support the presence of short-range order arrangements as opposed to specific inter-residue interactions.[3] Solution-state NMR and rheology studies reveal that gS-crystallin exhibits liquid properties until 400 mg mL^{-1}, at which the sample undergoes a sharp sol-gel phase transition. ^{15}N spin relaxation experiments reveal increased rigidity in local coiled regions induced by crowding effects. The affected regions are of high pathological relevance to the protein's remarkable structural stability. Clear understanding of human gS-crystallin behavior at native concentrations sets the foundation for further study. Thus, we can not only expand to lens protein mixtures (e.g., client-chaperone interactions), but also to cataract-associated mutants (e.g., influence of crowding effects on protein stability). Supported by NIH FG24428 and NIH R21EYEY035792.

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Jaewon Suk - University of California, Irvine
1201 Palo Verde Rd Irvine, CA, 92617 United States, Email: jaewos1@uci.edu

Lipid Regulation of Membrane Proteins as Observed by Solid State NMR

Benjamin J. Wylie, Jun Jang, Carver Rasberry, Sara Bannister, Duncan Chandler, Collin Borcik, Reza Amani, Evan van Aalst, Maryam Yekefallah

Indiana University Bloomington, Texas Tech University Lubbock

Lipid-protein coaction governs biological function and organization. The functional interplay of these bilayer components regulates the flux of ions, molecules, and information across the plasma membrane. Here I will describe the functional interactions between inward-rectifier K^+ (Kir) channels and chemokine G protein-coupled receptors (GPCRs) to their native lipid and ligand partners.

In Kir channels, ssNMR measurements, simulated annealing structure calculations, and coarse-grain molecular dynamics (CG-MD) we resolved an intricate allosteric network between the inner gate, outer gate,and intracellular Kir domain. This network is governed by positive anioniclipid-loading allostery. Our work shows that channel activity can be regulated by the cell through control of bilayer composition. This implies that the closed/inactivated state of the channel corresponds to a tense (T) state, and the open/activated state of the channel is the relaxed (R) state. Our structure of the activated R state is a fully conductive state of the channel. We also showed how bilayer cholesterol can competitively inhibit the channel. This shows how lipid-protein coaction acts as a critical gating mechanism and nucleator for bilayer heterogeneity and organization.

Activation of the CCR3 receptor by the CCL11 ligand is strongly influenced by membrane lipids. We discovered a direct correlation between bilayer cholesterol and increased agonist-triggered CCR3 signal transduction. Therein, we observed that the presence of cholesterol influences receptor structure to remodel activation pathway residue contacts and constrain conformational sampling favorable for CCL11 interaction. We solved a high-resolution structure of CCL11 at high-field (1.1 GHz). The ensemble exhibits not only more defined secondary structures compared to past reports, but also a less dynamic disulfide bonds and N-terminus. Ligand-receptor docking of our structure verifies the docking viability of our minimized average structure, resulting in the N-terminus of CCL11 properly docked to the orthosteric pocket of CCR3. This is complemented by ultra-high field ssNMR spectra of CCR3, where over 80% of backbone correlations are cleanly resolved in three-dimensional spectra.

Benjamin Wylie - Indiana University
800 E. Kirkwood Ave. Bloomington, Indiana, 47405 United States, Email: benwylie@iu.edu

a-Synuclein Membrane Binding with DNP NMR

Sahil Ahlawat,[1] Rania Dumarieh,[1] Dominique Lagasca,[1] Shubha Gunaga,[2] Faith Scott,[2] Frederic Mentink-Vigier,[2] Kendra Frederick[1]

UT Southwestern Medical Center, Department of Biophysics, Dallas, TX 75390Florida State University, National High Magnetic Field Laboratory, Tallahassee, FL 32310

a-Synuclein (a-syn) adopts multiple conformations ranging from an intrinsically disordered monomer, an a-helical membrane-associated state and ß-sheet structures during aggregation. The a-helical membrane-associated form is thought to play an important role in cellular function and toxicity during aggregation. However, despite its high affinity for membranes *in vitro*, direct evidence for membrane-bound a-syn inside cells remains limited, and it is not clear whether a-syn adopts this conformation under physiological conditions. Resolving this question is essential for understanding the functional and pathological roles of a-syn. DNP-enhanced solid-state NMR provides a unique approach to directly probe these interactions in cellular environments by enabling atomic-resolution measurements at endogenous concentrations. In particular, under DNP conditions, dipolar recoupling experiments such as ^{31}P–^{13}C/^{1}5N REDOR can be used to measure distances between a-syn and membrane phospholipids, providing direct evidence of membrane association. Here, we present initial results from *in vitro* model systems that establish the experimental framework for these measurements. Using uniformly ^{13}C, ^{1}5N-labeled lysine a-syn bound to nanodiscs, we reduce spectral overlap and obtain site-specific distance constraints using ^{31}P REDOR under DNP conditions. These measurements validate structural models in which lysine side chains interact with phospholipid head groups and define the geometry of a-syn–membrane interactions. This framework serves as a reference for ongoing in-cell studies aimed at determining whether a-syn adopts a membrane-bound conformation in its native cellular environment.

Sahil Ahlawat - UT Southwestern Medical Center
5323 Harry Hines Blvd Dallas, Texas, 75390 United States, Email: sahil.ahlawat@utsouthwestern.edu

Magnetic Resonance Studies of Paramagnetic and Metallic Battery Materials

Clare Grey

University of Cambridge, Yusuf Hamied Department of Chemistry, Cambridge, UK

This talk will describe recent studies to (i) understand the mechanisms underpinning Li metal DNP as applied to Li plating in anode-free and graphite-based batteries, (ii) apply Overhauser DNP more widely and (iii) use paramagnetic NMR and DNP methods to track defects in cathode materials and lithium-ion solid state electrolytes.

Clare Grey - University of Cambridge
Lensfield Road Cambridge, Cambridgeshire, CB2 1EW United Kingdom, Email: cpg27@cam.ac.uk

Mechanochemical Synthesis and Multinuclear Solid-State NMR Spectroscopy of Metal Coordination Compounds

Jazmine E. Sanchez,[1,2] Sean T. Holmes,[1,2] James S. Cohan,[1,2] Christine E. A. Kirschhock,[3] Eric Breynaert,[3,4] Danielle Laurencin,[5] Thomas-Xavier Métro,[5] and Robert W. Schurko.[1,2]

1. Department of Chemistry &; Biochemistry, Florida State University, Tallahassee, FL 32306
2. National High Magnetic Field Laboratory, Tallahassee, FL 32310
3. Centre for Surface Chemistry and Catalysis – Characterisation and Application Team, KU Leuven, 3001 Leuven, Belgium
4. NMR/X-ray platform for Convergence Research (NMRCoRe), KU Leuven, 3001 Leuven, Belgium
5. ICGM, Univ. Montpellier, CNRS, ENSCM, Montpellier, France

Over the past fifty years, overuse of antibiotics has led to resistant pathogens, reducing their effectiveness. Silver-containing coordination compounds show promise as antibacterial agents due to their excellent antibacterial properties. Mechanochemical preparation of metal coordination compounds has garnered recent interest due to a need for environmentally-friendly syntheses that are rapid, high-yielding, and scalable. Structural characterization of mechanochemically synthesized metal coordination compounds can be challenging since the products are typically microcrystalline powders. However, combining solid-state NMR spectroscopy, PXRD, and relativistic density functional theory calculations can help determine their structures through a method known as NMR crystallography (NMRX). Common NMR studies focus on ^{1}H, ^{13}C, and ^{15}N nuclei, but the potential of quadrupolar and heavy metal nuclei remains underexplored despite the rich structural information that they can provide. Herein, we discuss the synthesis and characterization of two silver-based coordination compounds, [Ag(R)$_n$NO$_3$] (R = 4- and 5-aminosalicylic acid; 4-ASA and 5-ASA), using PXRD and multinuclear SSNMR (i.e., ^{13}C, ^{15}N, and ^{109}Ag). The 4-ASA compound serves as a model to develop an NMRX-guided Rietveld refinement protocol leveraging CS and/or EFG tensors, which could be applied to other metal coordination compounds, including those containing copper or cadmium by using $^{63/65}$Cu and ^{113}Cd SSNMR to probe the metal centers and $^{35/37}$Cl SSNMR to probe the ligands. Additionally, mechanochemical isotopic labeling of the ligands in ^{17}O and subsequent analysis by ^{17}O SSNMR offers deeper insights into the bonding interactions between the metal ion and the organic ligand. This research aims to characterize structural and bonding motifs in metal coordination compounds, which in term could lead to the rational design of new antibacterial agents with valuable physicochemical or pharmacological properties.

Jazmine Sanchez - Florida State University
1102 N Bronough St Tallahassee, FL, 32303 United States, Email: sanchezjazzy1@gmail.com

Surface-Only NMR of Calcium Silicate Hydrate: Advancing Surface-Selective Methods to the Atomic-Level Surface Structure Of Cements

X. Ray Cowen,[1,2] Tristan Georges,[1] Karen Scrivener,[2] Lyndon Emsley[1]

1. École Polytechnique Fédérale de Lausanne, Laboratory of Magnetic Resonance, Institut des Sciences et Ingéniere Chemiques, 1015 Lausanne, Switzerland
2. École Polytechnique Fédérale de Lausanne, Laboratory of Construction Materials, Institut des Matériaux, 1015 Lausanne, Switzerland

Demand for cement, currently over 4 billion tonnes annually, is projected to continue to grow in the coming decades, driving the need for new, sustainable cements. The development of such cements necessitates a complete understanding of the structure of the main binding phase, calcium silicate hydrate (CSH). Nuclear magnetic resonance (NMR) spectroscopy has proven to be a powerful tool in the atomic-level study of CSH; from its first use in the 1980s,[1] to the observation of the later stages of the hydration reaction[2] or the determination of the bulk structure of CSH.[3] However, direct experimental probes of the surface structure remain elusive. The extremely thin nature of CSH (~5 nm), and the ubiquity of hydrogen atoms throughout the structure, makes the application of even traditional surface-selective NMR techniques impossible. Here, for the first time, we experimentally differentiate the surface structure from the bulk using new surface-only NMR methods. Through the combination of dynamic nuclear polarization (DNP) methods with selective deuteration, we isolate NMR signals from silicate units originating exclusively at the surface of CSH, thus allowing for characterization of the surface structure. This breakthrough allows for analysis of the surface of CSH and its variants to uncover connections between atomic structure and macro-scale properties.

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Ray Cowen - EPFL
Av. F.-A. Forel 2 Lausanne, VD, 1015 Switzerland, Email: ray.cowen@epfl.ch

Measuring, Calculating, and Overcoming Large Anisotropies in Energy Materials

M. A. Hope,[1] H. R. Loan,[1] R. J. Bragg,[1] C. F. Walton,[1] R. I. Walton,[1] A. J. D. Pauletto,[1] K. Petzall,[1] P. Gill,[2] A. J. Morris[2]

Department of Chemistry, University of Warwick, Coventry, CV4 7AL, U.K. School of Metallurgy and Materials, University of Birmingham, Birmingham, B15 2TT, U.K.

Anisotropic interactions can provide a wealth of information in solid-state NMR spectra, but also lead to experimental and computational challenges. Here, I will present three recent examples exploiting anisotropic NMR in the sphere of energy materials. 1) Metal–organic frameworks (MOFs) based on Sn(II) metal nodes have been proposed as anode materials in lithium-ion batteries. Sn(II) has a stereoactive lone pair which results in unusual MOF structures and causes a large ^{119}Sn chemical shift anisotropy (CSA). We measured the ^{119}Sn CSA of 6 Sn(II) carboxylate MOFs, with between 1 and 3 Sn sites per structure, using variable MAS and static wideline BRAIN-CP-WCPMG experiments. Comparing to DFT calculations, we find good agreement for the isotropic shift, but DFT systematically underestimates the CSA. By accounting for the anisotropic effect of the Sn(II) lone pair on the shielding tensor, the experimental CSAs can be accurately calculated. 2) Ag–Bi double perovskites are of interest as lead-free alternatives to halide perovskite optoelectronic materials, which can be tuned by halide mixing. ^{209}Bi NMR spectroscopy is sensitive to the local environment but suffers from severe quadrupolar broadening. Combining the UK's new 1.2 GHz spectrometer, fast magic angle spinning, and a sideband separation pulse sequence, all seven local [BiX_6] configurations can be distinguished in the ^{209}Bi NMR spectra of mixed chloride–bromide $Cs_2AgBi(Cl_{1-x}Br_x)_6$ ($0 = x = 1$) double perovskites. 3) Layered lead-halide perovskites can be used as coatings to improve the stability of photovoltaic devices. $^{79/81}$Br quadrupolar coupling is extremely sensitive to the local structure, but exploiting this is limited by both experimental and computational challenges. Combing NQR and high-field (>23T) ultra-wideline NMR experiments has enabled the $^{79/81}$Br quadrupolar parameters of several 2D lead bromide perovskites to be measured experimentally for the first time and used to benchmark DFT calculations.

Michael A. Hope - University of Warwick
Department of Chemistry, University of Warwick Coventry, Coventry, CV4 7AL United Kingdom, Email: michael.hope.1@warwick.ac.uk

Deciphering the Topology of Less Ordered Materials Using an NMR Assisted Approach

Brijith Thomas

New York University AbuDhabi, United Arab Emirates

Profound knowledge of the molecular structure and supramolecular organization of organic molecules is essential for understanding their structure–property relationships. In this talk, I will highlight the importance of unraveling the molecular structure and supramolecular organization of organic molecules to gain insights into their structure– property relationships. I will demonstrate how the structure of partially disordered systems can be elucidated through an interdisciplinary approach that integrates solid-state NMR, 3D electron diffraction (3D ED), and DFT calculations. The synergy between experimental and theoretical methods holds significant promise for investigating novel materials with unique properties that are challenging to study usingconventional techniques due to their inherent disorder. By effectively addressing these challenges, our methodology paves the way for new avenues in material characterization, driving exciting advancements in the field.

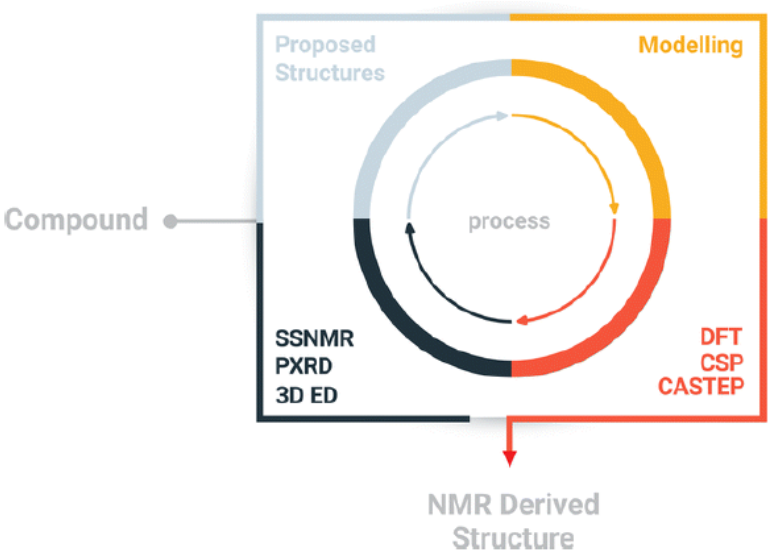

Fig 1: Schematic diagram of the structure determination approach. The approach combines complementary techniques like and solid-state NMR, powder X-ray diffraction and electron diffraction on a quantum mechanical platform to integrate the results.

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Brijith Thomas - New York University Abudhabi
C1 104, Newyork university Abudhabi Saadiyat Island, Abu Dhabi, `AbuDhabi United Arab Emirates, Email: brijiththomas@nyu.edu

Combining CSA and Dipolar recoupling reveals a dynamic window in filamentous phage capsids

Amir Goldbourt

School of Chemistry, Tel Aviv University

Ff Filamentous phages are one-micron long viruses containing a single-stranded DNA with ~8000 bases wrapped by ~3500 copies of a major coat protein, g8p. The structure of the phage shows that the capsid protein is mostly helical and strengthened by strong hydrophobic interactions. In order to assess the dynamic properties of g8p in the viral capsid, we used pseudo-3D experiments to measure ^{13}C and ^{15}N CSA, as well as backbone and sidechain C-N dipolar order parameters. These two complementary experiments have different upper-bound limits of their time scales. We find approximate static-limit CSA couplings (6 and 12 kHz for ^{15}N and ^{13}C, respectively) for most residues suggesting a rigid capsid on this time scale. On the other hand, the multiple REDOR curves, which were resolved using either single-quantum (DARR, RFDR) or double-quantum J-based spectroscopy, report on capsid motions on a time scale of ~1 kHz and on the highly dynamic N-terminus. Both CSA and C-N dipolar couplings are also shown to be excellent tools to characterize the dynamics involved in capsid-DNA interactions.

Amir Goldbourt - Tel Aviv University
Tel Aviv University, Ramat Aviv Tel Aviv, none, 6997801 Israel, Email: amirgo@tauex.tau.ac.il

Influence of Paramagnetic Relaxation Additives on DNP-enhanced MAS NMR

Ronja Roessler,[1] Kenneth Millow,[1] Bjoern Corzilius.[1,2]

1. Institute of Physical Chemistry, University of Rostock, 18059 Rostock, Germany
2. Department of Life, Light and Matter, University of Rostock, 18059 Rostock, Germany

In solid-state NMR spectroscopy, dynamic nuclear polarization (DNP) is one of the most prominent methods for generating hyperpolarization in order to enhance sensitivity. DNP is based on the transfer of polarization from the electron spin of a paramagnetic polarization agent (PA) to nuclear spin via hyperfine interaction (HFI). However, paramagnetic relaxation enhancement (PRE) induced by the PA often leads to compromised spectral resolution due to signal quenching of the nuclei close to the PA, giving rise to the occurrence of a 'blind sphere' around the PA. Yet, no quantitative model of paramagnetic relaxation under cryogenic conditions relevant for MAS DNP exists. In order to develop strategies for mitigation of this effect, we want to gain a deeper understanding of paramagnetic relaxation under the conditions typically encountered during MAS DNP NMR. To this end, we investigated the influence that the addition of paramagnetic salts (additives) has on DNP parameters. We performed MAS DNP measurements of standard DNP formulations (1 M ^{13}C-urea in 60:30:10 d_8-glycerol/H_2O/D_2O with 10 mM AMUPol as PA), to which we added various paramagnetic salts in varying concentrations. Here, we find that the paramagnetic additives lead to a lower steady-state signal enhancement, while the polarization build-up rate was increased. The strength of this effect depends on the spin quantum number *S* of the additive as well as on its concentration, with the tendency of lower spin quantum numbers and higher concentrations leading to a stronger effect. For some additives, also the effect of peak broadening has been evaluated. Our results will aid the development of a quantitative model of paramagnetic relaxation under MAS DNP conditions which is crucial for further developments for site-specific DNP. Furthermore, it provides important information for MAS DNP of paramagnetic (biological) materials, such as heme-containing tissue or blood.

Ronja Roessler - University of Rostock, Germany
Albert-Einstein-Straße 27 Rostock, Mecklenburg-Vorpommern, 18059 Germany, Email: ronja.roessler@uni-rostock.de

Nanosecond Electron Spin Dynamics in Diamond Probed by Pulsed DNP at 7 T

Nevzorov, Alexander A., Milikisiyants, Sergey, Marek, Antonin, and Smirnov, Alex I.

Department of Chemistry, North Carolina State University, 2620 Yarbrough Drive, Raleigh, NC 27695-8204, U.S.A

We report on an electron-nucleus correlation experiment demonstrating nanosecond scale transient oscillations arising from direct Dynamic Nuclear Polarization (DNP) transfer from P1 centers to the nearby ^{13}C spins in a high-pressure high-temperature diamond crystal. These oscillations detected by the bulk ^{13}C spins cannot be explained by conventional spin-diffusion because of large hyperfine mismatches between the remote and directly bonded ^{13}C. Thus, a new model based on electron-pair relayed mechanism has been proposed. Closed-form expressions for the resonant four-spin transitions have been derived yielding the transfer efficiency as a function of the electron-electron exchange coupling and their frequency offset. These experiments were made possible by our unique spectrometer capable of performing time-domain ESR as well as both pulsed and continuous-wave DNP at the 7 T magnetic field. In combination with an extended interaction klystron producing up to 140 W peak output power, the spectrometer also features an integrated ESR/NMR probehead incorporating all-dielectric photonic band-gap resonators for boosting mm-wave fields at the sample, which are remotely tunable by a piezoelectric stage. The transverse electronic B_{1e} fields of 75-150 MHz generated at the sample allow for performing pulsed NOVEL DNP, which was previously inaccessible at such field/frequencies even when using high-power gyrotrons. The nanosecond magnetization buildup demonstrated using this spectrometer paves the way to room temperature DNP by dramatically reducing the average mm-wave power deposited into the sample. Furthermore, these recent technological and theoretical advances greatly enhance the potential of pulsed DNP for transferring and detecting hyperpolarization originating from short-lived electronic states to nuclear spin reservoirs having much longer relaxation times. Supported by NSF DBI 2311042.

Alexander Nevzorov - North Carolina State University
2620 Yarbrough Drive Raleigh, North Carolina, 27695-8204 United States, Email: alex_nevzorov@ncsu.edu

Solid-State NMR and DNP Investigation of PFAS Binding in Zr-Based MOFs

Kunyu Wang,1 Duhan Zhang,2 Yaojun Zeng,1 Ashley Beers,2 Jochem Struppe,3 Daniel Banks,3 James Kempf,3 Yifan Quan,2, * and Shu Yang1

1Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA 19104, USA
2Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA
3Bruker Biospin, Billerica, MA 01821, United States

Metal-organic frameworks (MOFs) are crystalline materials with nanosized pores for transporting energy and matters, based on the interconnection of metal nodes and organic liagnds. Engineering their pore environments at nanoscale can facilitate the ingress of guest molecules and broaden their practical applications. Herein, we have developed a Zr-based MOF consisting of accessible binding sites to accommodate per- or poly-fluoroalkyl substance (PFAS), which are emerging contaminants widely
observed in drinking water in the US. Benefiting from the hierarchical porosity of the MOF, it is able to remove > 90% perfluorooctanoic acid (PFOA) in water within 1 min, which paves the pathway for real-world applications in water purification. Furthermore, the strong coordination bond between Zr atoms and carboxylate groups ensures the high chemical stability of the MOF, which can remain robust
in strong acid for 24 hours.
To directly probe host-guest interactions, we performed solid-state NMR experiments at 500 MHz using a 1.3 mm HFX MAS probe. 1H MAS and 13C CP-MAS spectra of PFOA-loaded MOF suggest deprotonation upon adsorption and formation of coordinated carboxylate species, with additional stabilization via hydrogen bonding. Two-dimensional 19F-1H HETCOR experiments provide direct spatial correlations between MOF hydroxyl protons and both CF2 and CF3 groups. These data support a model in which PFOA is confined within the MOF pores, anchored via its headgroup to Zr6 clusters, while the fluorinated chain extends into the pore and interacts with the framework. This host-guest structure is further supported by density functional theory (DFT) calculations.
19F DNP is a powerful approach to studying PFAS adsorption. DNP experiments were performed at 400 MHz using AMUPOL as the polarizing agent. A 1H enhancement of e ~ 32 was achieved, whereas the 19F enhancement remains limited (e ~ 3), underscoring the need for HFX probe to improve sensitivity in 19F-detected experiments.

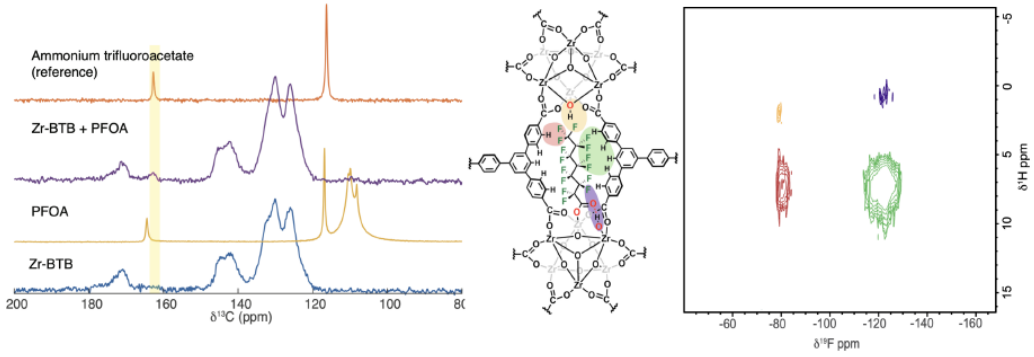

FIG. 1: Solid-state NMR characterization and proposed binding mode of PFOA within the Zr-based MOF. (**Left**) ^{13}C CP-MAS spectra. The shift of the PFOA carboxyl carbon upon adsorption indicates deprotonation and coordination to Zr_6 clusters. (**Center**) Schematic illustration of the host–guest binding configuration, showing coordination of the PFOA carboxylate headgroup to open Zr sites and confinement of the fluorinated chain within the pore. (**Right**) ^{19}F-^{1}H HETCOR spectrum, revealing spatial correlations between MOF hydroxyl protons and CF_2/CF_3 groups.

Yifan Quan - University of Pennsylvania
231 S. 34 Street Philadelphia, PA, 19104 United States, Email: yquan@sas.upenn.edu

A Proposed NMR Correction to the Crystal Structure of Cefdinir Anhydrate

J. K. Harper,[1] E. C. Heider,[2] L. Mueller,[3] A. Thome,[3] and J. Hartman.[3]

1University of Utah, Department of Chemistry, Salt Lake City, UT, 84112, 2Utah Valley University, Department of Chemistry, Orem, UT, 84058, 3University of California, Riverside, Riverside, CA, 92521

In numerous studies over the past 30 years, NMR crystallographic methods have demonstrated the ability to improve existing crystal structure. These improvements usually come from small adjustments to atom positions and bond lengths and commonly involve hydrogens. More impactful changes have been reported by a much smaller number of studies and include the identification of tunneling hydrogens, adjustment of protein backbone conformation and corrections to non-hydrogen atom positions. The present study builds upon these results by employing solid-state NMR methods to identifying a problematic bonding arrangement in crystal structure of the antibiotic cefdinir anhydrate. An alternative bonding arrangement is proposed that creates a previously unreported tautomer of cefdinir. This tautomer is a zwitterion and exhibits an improved fit to the experimental x-ray powder diffraction pattern and a more favorable lattice energy. The zwitterion also significantly improves agreement between experimental and computed ^{13}C and ^{15}N chemical shift tensors. The thiazole tautomer proposed has not yet been considered as a contributor to biological activity studies of cefdinir and may provide new insights into the mechanism of activity.

James Harper - University of Utah
315 S. 1400 E. Salt Lake City, Utah, 84112 United States, Email: James.Harper@utah.edu

Fast and accurate NMR crystallography with Machine Learning Interatomic Potentials

Shubha S. Gunaga,[1] Robert W. Schurko, [1,2] Sean T Holmes,[1,2] Frederic Mentink-Vigier[1,2]

[1]National High Magnetic Field Laboratory, Florida State University, 1800 E. Paul Dirac Dr, Tallahassee, FL, 32310, USA.
[2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306, USA.

Nuclear magnetic resonance (NMR) crystallography is a robust method for structure determination, but its reliance on costly density functional theory (DFT) for geometry refinement limits its speed and accessibility. While machine learning tools such as ShiftML3 predict magnetic shieldings in seconds,[1] they still require high-quality input geometries, typically obtained from slow DFT optimizations. Herein, we demonstrate that machine learning interatomic potentials (MLIPs) eliminate this bottleneck for organic crystals. Interestingly, models trained on gas-phase molecules at the hybrid ?B97M-V level (OMol25 dataset)[2] — such as UMA-*omol*[3] and MACE-Polar-1[4] — deliver structural quality rivaling hybrid periodic-DFT, without requiring large computational resources. The resulting MLIP–ShiftML3 workflow reduces computational cost by at least three orders of magnitude relative to DFT-based methods, making high-accuracy NMR crystallography accessible without HPC infrastructure, and opening the door to rapid molecular dynamics simulations at the hybrid DFT level. Combined with sensitivity enhancement via dynamic nuclear polarization (DNP), we demonstrate the approach on L-histidine, extracting the ^{13}C and ^{1}5N chemical shift tensors, and ^{1}H chemical shifts, at natural isotopic abundance and discriminating between its monoclinic and orthorhombic polymorphs.
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Frederic Mentink-Vigier - National High Magnetic Field Laboratory
1800 E Paul Dirac Dr Tallahassee, Florida, 32310-3706 United States, Email: fmentink@fsu.edu

Determination of Atomically Precise Models of CdSe Quantum Dots Using DNP-Enhanced REDOR Solid-state NMR Spectroscopy.

Anuluxan Santhiran,[1, 2] Jie Zhu,[4] Xueqian Kong,[5] Xiaogang Peng,[4] Javier Vela,*[1, 2] Frédéric A. Perras,*[1, 2, 3] and Aaron J. Rossini*[1, 2]

[1]Division of Materials Science and Engineering, Ames National Laboratory, Ames, Iowa, USA 50011.
[2]Department of Chemistry, Iowa State University, Ames, Iowa, USA 50011.
[3]Division of Chemical and Biological Sciences, Ames National Laboratory, Ames, Iowa, 50011, United States.
[4]Key Laboratory of Excited-State Materials of Zhejiang Province and Department of Chemistry, Zhejiang University, Hangzhou, 310027, China.
[5]Institute of Translational Medicine, Shanghai Jiao Tong University, Shanghai, 200240, China.

Quantum dots (QDs) have been widely investigated due to their unique optoelectronic properties. Their photophysical properties can be modulated and optimized by surface ligand or by growing an inorganic shell. Therefore, there is a critical need to understand the atomic-level structure of QD surfaces and interfaces. Here, we show that multinuclear rotational-echo double-resonance (REDOR) solid-state NMR experiments can be used to measure heteronuclear distances in CdSe QDs. We have performed DNP-enhanced $^{13}C^{77}Se$, $^{77}Se^{13}C$, and $^{13}C^{111}Cd$ REDOR experiments to probe the heteronuclear distances between carbon, selenium, and cadmium. The INTERFACES[1] computer program can be used to quickly and accurately simulate the REDOR dephasing curves. Based upon this analysis, we conclusively show that the QDs have a zinc blende crystal structure with a dense network of chelating carboxylate ligands coordinated to surface Cd atoms. These experiments can also be applied to determine precise structural models of CdSe/CdS core/shell QDs, where REDOR enables the ratio of sulfur and selenium atoms within the first few layers of each QD to be determined.
1. Cunningham, J. and Perras, *J. Magn. Reson. Open*, 2022, *12*, 100066.

Anuluxan Santhiran - Iowa State University
Pammel Drive Ames, IA, 50011 United States, Email: anuluxan@iastate.edu

Exploiting High-Spin Gd(III) Central Transition for reduced-power Pulsed DNP (NOVEL)

Zhenfeng Pang,[1] Marcel Levien,[2] Jean-Paul Amoureux,[3] Lyndon Emsley,[4] Marinella Mazzanti,[2] Hervé Vezin,[5] Kong Ooi Tan,[1]

[1]Chimie Physique et Chimie du Vivant (CPCV), UMR 8228, Département de Chimie, École Normale Supérieure, PSL University, Sorbonne Université, CNRS, 75005 Paris, France.
[2]Group of Coordination Chemistry, Institut des Sciences et Ingénierie Chimiques, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.
[3]Univ. Lille, CNRS, Centrale Lille, Univ. Artois, UMR 8181, UCCS - Unité de Catalyse et Chimie du Solide, F-59000 Lille, France.
[4]Laboratory of Magnetic Resonance, Institut des Sciences et Ingénierie Chimiques, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.
[5]University of Lille, CNRS UMR 8516 - LASIRE - Laboratoire de Spectroscopie pour les Interactions la Réactivité et l'Environnement, Lille 59000, France.

Dynamic Nuclear Polarization (DNP) is a powerful approach for enhancing NMR sensitivity, yet high-field implementations of pulsed techniques like NOVEL are often hindered by the extreme microwave power required. This study proposes utilizing the high-spin Gd(III) (S=7/2) central transition to bypass these limitations. Theoretically, the effective nutation frequency for the ±1/2 transition in half-integer spin systems is scaled by S+1/2, which for Gd(III) results in a 16-fold reduction in power requirements compared to S=1/2 radicals. Preliminary X-band (0.35 T) results demonstrated a 9-fold power reduction, though enhancement factors were limited by the broad central transition linewidth at low fields. By transitioning to higher fields (Q band and W-band), we expect the narrowed linewidth will allow better DNP performances. Additionally, we also examined broadband and adiabatic "BRAIN-NOVEL" sequences. The latter, employing frequency-chirped WURST pulses, exhibits superior robustness against microwave power inhomogeneity. Additionally, the rapid $T_{1e?}$ relaxation of Gd(III) at low temperatures accelerates the DNP build-up process. We present experimental progress on ^{1}H pulsed DNP, establishing a new regime for high-field sensitivity enhancement.

Kong Ooi Tan - École Normale Supérieure
24 Rue Lhomond Paris, Paris, 75005 France, Email: kong-ooi.tan@ens.psl.eu

Dynamic Nuclear Polarization with 1.3 mm Diameter Diamond Rotors

Nicholas Wiesner[1], Jiaming Liu[2], Ravi Shankar Palani[1], Samuel Strymish[1], Neil Gershenfeld[2], Robert G. Griffin[1]

[1]Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, United States
[2]Center for Bits and Atoms, Massachusetts Institute of Technology, Cambridge, MA 02139, United States

Magic angle spinning (MAS) nuclear magnetic resonance (NMR) has revolutionized structural biology due to the development of methods to precisely determine bond lengths and torsion angles in medicinally relevant solids such as Aß. Hydrostatic air bearings stabilize small rotors allowing for rotational frequencies over 200 kHz, greatly improving resolution for solid samples. Complementing this technique is dynamic nuclear polarization (DNP) where electron polarization is transferred to local nuclei mediated by microwave excitation. Signal enhancements of ~10^2 are currently routinely achieved. While these techniques can greatly improve resolution and sensitivity, they come with significant operational challenges. The high spinning frequency of MAS rotors may induce structural failure leading to a loss of the sample and causing serious damage to the MAS stator and RF circuitry. Additionally, thick rotor walls absorb microwave power attenuating high DNP enhancements. Currently, most MAS rotors (0.4 mm ? 3.2 mm diameters and larger) are fabricated from zirconia which has high durability but low thermal conductivity and microwave transmissibility. Sapphire rotors, on the other hand, exhibit improved microwave transmissibility and thermal conductivity but low durability. Because sapphire is fragile, rotor diameters are currently limited to = 3.2 mm. In recognition of these drawbacks, our group has recently fabricated 0.7 mm diameter rotors from single crystal HPHT diamond which displays better microwave transmissibility, tensile strength, and thermal conductivity than either of the other two materials.[1] This work includes both the creation of larger, 1.3 mm diamond rotors as well as the first ever DNP experiments to be performed with diamond rotors showing viability as an optimal rotor material.

Schaffer et. al., J. Magn. Res., 2025, *52*, 435.

Nicholas Wiesner - Massachusetts Institute of Technology
77 Massachusetts Avenue Cambridge, Massachusetts, 02139 United States, Email: wiesnern@mit.edu

Solid-State NMR and DNP Reveals Dynamic Lignin-Carbohydrate Architectures Across Plant Development and Carbon Cycling

Tuo Wang[1], Priya Sahu[1], Peng Xiao[1], Debkumar Debnath[1], Shubha S. Gunaga[2], Faith Scott[2], Jayasubba Yarava[1], Frederic Mentink-Vigier[2]

[1] Department of Chemistry, Michigan State University, East Lansing, Michigan 48824, United States
[1] Department of Chemistry, Michigan State University, East Lansing, Michigan 48824, United States
[2] National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, United States

Lignocellulosic biomaterials constitute the largest renewable carbon reservoir on Earth and underpin sustainable materials, bioenergy production, and long-term carbon sequestration. However, resolving their native molecular architecture remains challenging due to structural heterogeneity and limited spectroscopic sensitivity. Here we integrate ^{13}C- and ^{1}H-detected multidimensional solid-state NMR with DNP-enhanced techniques to achieve rapid, high-resolution characterization of intact plant cell walls and complex soil organic matter. These approaches enable in situ mapping of lignin-polysaccharide interactions and precursor-resolved tracking of lignin biosynthesis with substantially improved sensitivity and spectral resolution. Our results reveal that lignin-carbohydrate contacts in plant stems are developmentally staged, with acetylated xylan preferentially associated with syringyl-rich lignin in mature tissues, while methyl-esterified pectin interacts with guaiacyl lignin during early wall formation. Precursor-specific isotope labeling further uncovers distinct routing of phenylalanine and tyrosine into lignin substructures in grasses, indicating metabolic plasticity in polymer assembly. Extending these methods to saline wetland soils formed by degradation of grass residuals identifies parallel pathways of carbon persistence, where preserved aromatic and carbohydrate cores coexist with decomposition-repolymerization products. These studies establish sensitivity-enhanced solid-state NMR as a powerful platform for elucidating lignin-centered molecular networks from biosynthesis to long-term carbon fate.

Tuo Wang - Michigan State University
578 S. Shaw L East Lansing, Michigan, 48824 United States, Email: wangtuo1@msu.edu

Decoding Early Mineralization and Surface Layer Formation of Bone Mimetic Apatite Using Complementary Solution and Solid-State NMR

Cohen Lilian(1), Meizlik-Rothstein Shachar(1), Julian Holzinger(2), Barak Sharon(1), Robert Konrat(2), Goobes Gil(1)

1. Department of Chemistry and Center for Nanotechnology and Advanced Materials, Bar-Ilan University, Israel
2. Department of Structural and Computational Biology, University of Vienna, Austria

It is now common knowledge that order and crystallinity are intimately coupled to disorder in the bio composite structure of bone conferring some of the tissue's essential mechanical properties. The mechanisms through which bone's inorganic material, apatite ($Ca_5(PO_4)_3OH$), crystallizes, a key step to bone proper function, are intensively scrutinized. At the same time, the formation of disordered mineral layers coating individual apatite crystals are enigmatic and challenging to underpin. We have systematically characterized layers with intermediate dis/order residing between the crystal and the outer amorphous film. We show that they are controlled by non-collagenous proteins. Spectrally filtered MAS NMR measurements vividly unveil the impact of these proteins on characteristics of these interphases.
Osteocalcin and osteopontin also intervene and regulate events at the other end of mineral formation, at early stages of ion clustering that precedes nucleation of amorphous phases and crystals. Time resolved solution ^{31}P NMR of apatite precursor ions during in situ mineralization in the NMR tube are used to follow rates of mechanistic steps in precipitation events and how they are influence by the proteins.
Osteopontin, an intrinsically disordered non-collagenous bone protein (NCP) and osteocalcin, modulate formation and properties of bone mineral, yet their mechanistic roles during the earliest stages of mineralization remain unclear. We induced hydroxyapatite mineralization in situ in NMR tubes and monitored phosphate–calcium association into polymeric precursor assemblies, and their conversion into pre-crystalline amorphous particles using time-resolved high-resolutionP solution NMR. Kinetic analysis of protein-dependent spectral variations—examined for each protein individually and in combination—distinguishes nucleation of precursor assemblies from growth of amorphous particles and reveals that osteocalcin and osteopontin exert differential control, selectively retarding or accelerating specific stages of particle evolution prior to crystallization. Complementary MAS NMR of hydroxyapatite formed in the presence of the two proteins shows that they also regulate the formation and composition of disordered mineral layers that coat hydroxyapatite crystallites, affecting water and inorganic ion environments implicated in remodeling. Together, the data support a mechanistic picture in which NCPs shape mineral outcome by directing early ionic clustering pathways and by modulating subsequent amorphous-to-crystalline transitions and surface layer formation.

Gil Goobes - BAR ILAN UNIVERSITY
1 MAX AND ANNA WEB ST Ramat Gan, Center, 5290002 Israel, Email: gil.goobes@biu.ac.il

NMR-Assisted Crystallography of Aspartate Aminotransferase: Protonation States and Catalytic Mechanism

Paula M. Magat[1], Jacob B. Holmes[1], Christopher G. Williams[1], Rittik K. Ghosh[1], Leonard J. Mueller[1]

[1] University of California, Riverside, Department of Chemistry, Riverside, CA 92521

Pyridoxal-5'-phosphate (PLP)-dependent enzymes comprise approximately 4% of all classified enzymes and catalyze a remarkable range of reactions, including transamination, racemization, decarboxylation, and carbon rearrangements.[1] Despite their prevalence and importance, the molecular origins of reaction specificity among PLP-dependent enzymes remain incompletely understood.[2] Increasing evidence suggests that protonation states within the active site play a central role in controlling catalytic function.[3] Aspartate aminotransferase (AAT), a model PLP-dependent enzyme, utilizes finely tuned protonation equilibria to stabilize carbanionic intermediates during the reversible transamination of dicarboxylic amino acids and ketoacids.[4] However, direct determination of hydrogen atom positions and protonation states remains challenging using conventional structural biology techniques.

To address this limitation, we employ NMR-assisted crystallography, integrating solid-state NMR spectroscopy, diffraction-based structural methods, and quantum chemical calculations to investigate the active-site chemistry of AAT at atomic resolution. High-resolution ^{13}C and ^{15}N solid-state NMR spectrum were acquired using a Bruker CryoMAS probe, whose exceptional sensitivity enabled the detection and assignment of key isotopically labeled sites within the PLP cofactor, substrate analogs, and active-site residues. The enhanced signal-to-noise afforded by the CryoMAS provided critical chemical-shift information from ionizable groups, particularly the Schiff base and pyridine nitrogens, allowing protonation states and substrate-induced perturbations to be monitored in detail.

Experimental chemical shifts were combined with first-principles quantum chemical calculations and cluster models derived from crystallographic structures to evaluate candidate protonation-state models. This integrated approach refines structural descriptions of short-lived catalytic intermediates, improves hydrogen localization, and reveals how active-site protonation governs PLP reactivity and reaction specificity. Together, these results provide a chemically detailed framework for understanding PLP-mediated transamination and establish a foundation for future enzyme engineering, mechanistic studies, and rational inhibitor design.

Paula Magat - University of California, Riverside
501 W Big Springs Rd. Riverside, CALIFORNIA, 92521 United States, Email: pmaga003@ucr.edu

NMR-Assisted Crystallography of Aspartate Aminotransferase: Protonation States and Catalytic Mechanism

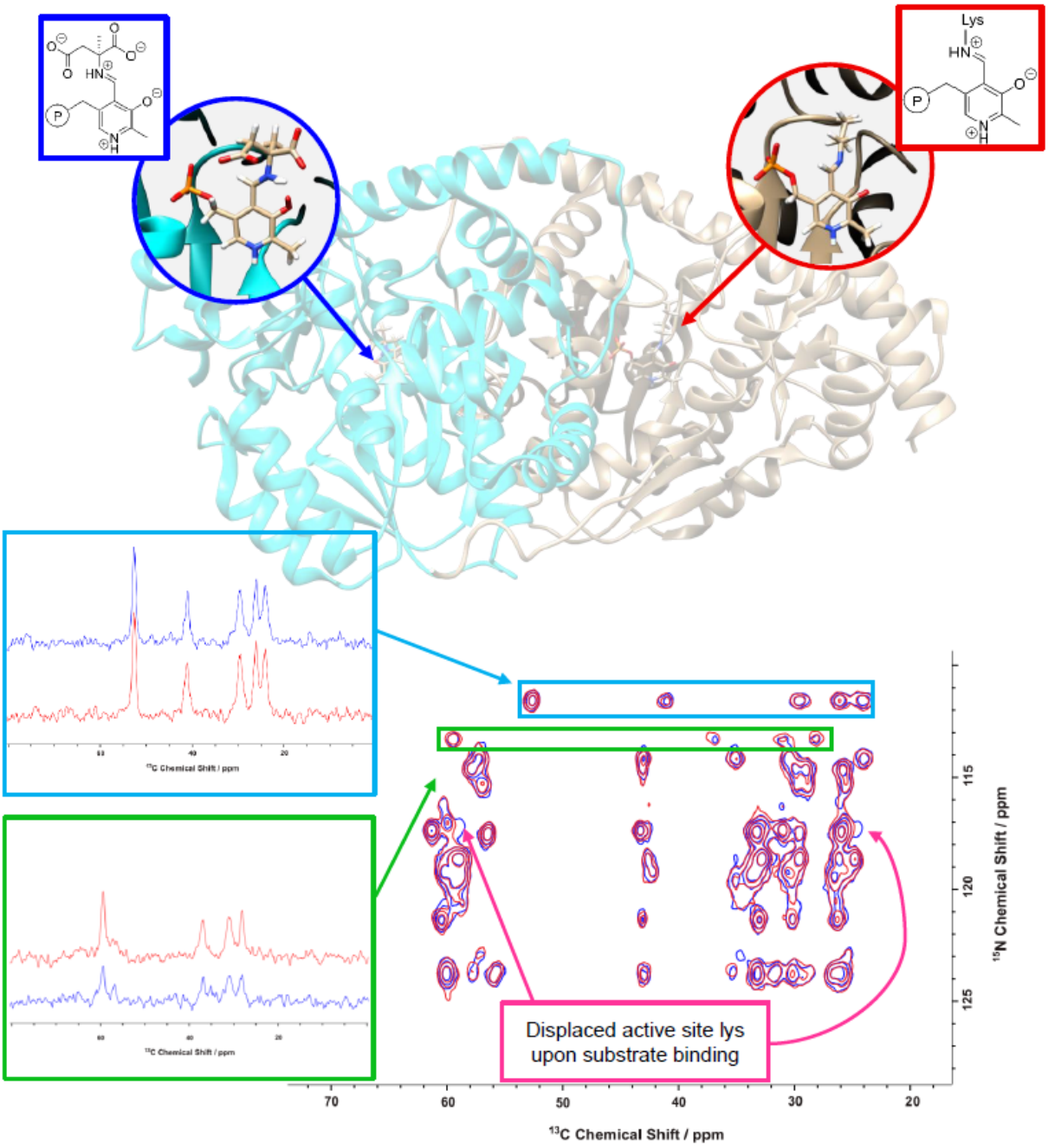

Figure 1: Joint x-ray/neutron structure of AAT asymmetric homodimer (PDB 5VJZ).[5] 2D NC spectra of [^{13}C, ^{15}N]-Lys labelled AAT showing correlations from amide backbone to side chain carbons. Loss of intensity in the active site lysine (green box), with respect to the other lysine residues (blue box) indicates reaction with substrate analogue, 2-methylaspartate.

Cryogen-free magnets for solid-state MAS NMR at multiple magnetic fields

Eugeny Kryukov[1], Alexander Karabanov[1], Denis Langlais[1], Dinu Iuga[2], Shashwata Moitra[3], Danielle Portugal[3], and Jeremy Good[1].

1. Cryogenic Ltd, London, UK
2. University of Warwick, Department of Physics, Coventry, UK
3. Cryogenic US LLC, Denver, USA

Cryogen-free systems (besides being free from the expensive liquid helium consumption) have several advantages compared with their conventional liquid helium counterparts: they are more compact, enable the top loading of the probe and can be used at different magnetic fields. We demonstrated that cryogen-free magnets provide the magnetic field homogeneity and stability well within the typical requirements for solid-state MAS NMR[1]. We developed a method to reduce the post-ramp field settling time down to an hour. That enables one to use the magnet at different fields without compromising the spectral resolution[2]. Recently, we discovered that some magnets accumulate eddy currents in their windings when they are ramped. These currents can significantly affect the magnetic field homogeneity, especially when the field is reduced from the maximum designed. We found a method to remove the eddy currents to restore the magnet homogeneity.

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2. Kryukov et al, SSNMR, 2020, 109, 101684.

Denis Langlais - Cryogenic US LLC
1327 Bexton St Charlotte, North Carolina, 28273 United States, Email: shashwata@cryogenic-usa.com

Probing the limits to refocusing nuclear spin dynamics

Shreyan Ganguly,[1] Chandrasekhar Ramanathan.[1]

1. Dartmouth College, Department of Physics and Astronomy, Hanover NH 03755

Out-of-Time-Ordered Correlators (OTOCs) provide a measure of how a local perturbation propagates through an interacting quantum system. They can potentially be used to study many problems in science, such as characterizing phases of matter and the thermalization of isolated quantum systems. The NMR multiple-quantum coherence (MQC) experiment is a version of an OTOC measurement. It has been suggested that such NMR OTOCS could improve large-scale molecular structure determination[1,2]. A key requirement for exploiting such OTOCs is that the large multi-spin correlations that build up during the NMR experiment have long coherence times and remain controllable. Refocusing the many-body dynamics of a system with high fidelity is key to OTOC measurements. In dipolar-coupled nuclear spin systems this refocusing is done via collective control of the spins. Here we characterize the fidelity of such refocusing and explore the sensitivity of OTOC dynamics to applied perturbation. We experimentally study the growth of MQC correlations in different systems and complement the experimental studies with numerical simulations. High sensitivity to small perturbations serves as a proof of failure of refocusing ability in the system and may establish bounds on the efficacy of OTOC-based studies in these systems. Supported by the Gordon and Betty Moore Foundation, grant DOI 10.37807/GBMF12251 and by Google LLC.
O'Brien et al. PRX Quantum, 3 030345 (2022).Zhang et al. www.arXiv.org:quant-ph/2510.19550.

Chandrasekhar Ramanathan - Dartmouth College
6127 Wilder Laboratory Hanover, NH, 03755 United States, Email: sekhar.ramanathan@dartmouth.edu

Linking Structure, Dynamics, and Reactivity in Energy Storage Materials through Operando Solid-State NMR and Relaxometry

Gillian R. Goward, Emma M. Magee, Aiman Quadiri, Cameron A. Gurwell, Honey Patel, Olivia Velenosi, Taiana L. E. Pereira, Ramesh C. Sahoo, Kevin J. Sanders

McMaster University, Department of Chemistry &; Chemical Biology, Hamilton, ON Canada L8S 4L8

Understanding the complex interplay between structure, ion dynamics, and interfacial reactivity remains a central challenge in the development of next-generation electrochemical energy storage systems. Solid-state NMR (ssNMR) spectroscopy offers unique capabilities to probe these processes across length and time scales, particularly under realistic operating conditions. In this talk, we highlight recent advances from our group that leverage multinuclear, *operando*, and electrochemically integrated NMR approaches to directly correlate local chemical environments with macroscopic battery performance. We demonstrate the use of *operando* ^{7}Li NMR spectroscopy via a parallel plate resonator configuration[1] to quantify lithium plating in graphite and silicon–graphite composite anodes under fast-charging and low-temperature conditions.[2,3] These studies reveal how temperature-dependent transport limitations promote metallic lithium formation, while compositional modifications influence plating tendency and improve reversibility. Insights into the relative kinetics of graphite intercalation versus Si-Li alloy formation are revealed. Building on this, we introduce a three-electrode *operando* NMR platform that decouples electrode potentials, enabling direct identification of the onset of lithium plating and quantification of reversible versus irreversible metallic lithium. Beyond lithium-ion systems, we show how *in situ* ^{1}H NMR can exploit paramagnetic relaxation effects to quantitatively track Mn^{2+} dissolution in aqueous Zn–MnO_2 batteries.[4,5] These measurements reveal that dissolution–redeposition is not merely a degradation pathway, but a dominant reversible charge storage mechanism. Changes in this behaviour with electrolyte composition and cathode particle size reveal that the NMR method provides reproducible diagnostic insights. These studies establish a unified strategy: combining tailored NMR methodologies, advanced cell designs, and quantitative analysis permits connecting local structure and dynamics with electrochemical function. This approach provides new mechanistic insights into interfacial processes, degradation pathways, and performance limitations across diverse battery chemistries. More broadly, it highlights the growing role of *operando* ssNMR as a cornerstone technique for guiding the design of next-generation energy storage materials.

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5. Miliante *et al.*, arXiv :2602.13116

Gillian Goward - McMaster University
1280 Main St. West Hamilton, ON, L8S 4G8 Canada, Email: goward@mcmaster.ca

Solid-state NMR spectroscopy of the platinum group elements and their replacements: experimental and computational advances

Sean T. Holmes,[1,2] Sara Termos,[1,2] Robert B. Smith,[1,2] Dominic C. Chantra,[1,2] Jazmine E. Sanchez,[1,2] Yijue Xu,[1] Adam B. Philips,[3] Alberto Fernández-Alarcón,[3] James J. Kimball,[1,2] Adam R. Altenhof,[1,2] Jochen Autschbach,[3] Robert W. Schurko[1,2]

1. National High Magnetic Field Laboratory, Tallahassee, FL 32310
2. Department of Chemistry & Biochemistry, The Florida State University, Tallahassee, FL 32306

The platinum group elements (PGEs), which include Rh, Ru, Pd, Os, Ir, and Pt, are widely used in catalysts, optical devices, sensors, alloys, and many other advanced materials. Because of their distinct electronic valence structures, PGEs engage in unique covalent donation bonding with a variety of ligands. Donation bonding may supersede other factors like atomic radii, electrochemical properties, preferred oxidation states, and coordination environments, which impacts the structure and reactivity of PGE coordination compounds, with the degree of covalent and ionic bonding character influencing emergent physicochemical properties and functionality. The combination of solid-state NMR (SSNMR) spectroscopy and density functional theory (DFT) calculations affords a powerful avenue into understanding this bonding, potentially enabling significant advances in the study of PGEs. In this talk, we discuss ongoing work to acquire ^{103}Rh and ^{99}Ru SSNMR spectra of coordination compounds with unprecedented signal-to-noise and uniformity using advanced pulse sequences and fields up to 36 T. Experimental chemical shift and EFG tensors obtained from these measurements are interpreted using state-of-the-art relativistic DFT calculations. Analyses of these tensors in terms of contributions from individual localized orbitals permits exploration of their relationships to structure and bonding. Additionally, these methods are applied to other transition metal such as Co and Cu to understand what makes them distinct from the PGEs. The combination of these experimental and computational methods lends deep insight into PGE-ligand bonding, possibly enabling the design of new coordination compounds with similar functionality, yet containing cheap and abundant replacement metals and/or ligands. Supported by U.S. Department of Energy, DE-SC0022310.

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Sean Holmes - Florida State University
1800 E Paul Dirac Dr Tallahassee, FL, 32310 United States, Email: sholmes2@fsu.edu

A ^{1}H NMR Investigation of a Birnessite-like MnO*x* Electrode Material

Mark O. Bovee,[1] Christopher A. Klug,[1] Eliana S. Dolven-Miller,[2] Ryan H. DeBlock,[1] Zoey Warecki,[3] Zachary G. Neale,[1] Debra R. Rolison,[1] and Jeffrey W. Long[1]

1. Chemistry Division, U.S. Naval Research Laboratory, Washington, DC, USA
2. Science and Engineering Apprenticeship Program, U.S. Naval Research Laboratory, Washington, DC, USA
3. Materials Science and Technology Division, U.S. Naval Research Laboratory, Washington, DC, USA

Lithium-ion battery technology dominates the rechargeable energy-storage device market;[1] however, flammability[2] and supply chain[3] concerns motivate the search for complementary alternatives.Aqueous electrochemical devices that incorporate alkali salt electrolytes and manganese oxide (MnO*x*) electrode materials can address these issues, but both the electrolyte's cations and protons can insert into these devices' MnO*x* electrode during charge storage. Because protons generally have higher solid-state mobilities, in some cases it may be advantageous to prioritize their involvement when optimizing electrochemical performance.[4] This underscores the importance of understanding how protons are incorporated into these materials and their behavior during the energy storage process.Herein, we utilize static ^{1}H NMR spectroscopy to investigate the structural environments available to protons in a birnessite-like manganese oxide electrode formed through the electroless deposition of MnO*x* onto carbon nanofoam paper (MnO*x*@CNFP). Its ^{1}H spectrum contains two features attributed to water molecules at different distances away from paramagnetic Mn ions in the material's octahedral MnO_6 layers. Additionally, selective inversion measurements reveal chemical exchange occurs between these environments in a multistep process, and measurements of MnO*x*@CNFP at different orientations with respect to B_0 demonstrate the influence of bulk magnetic susceptibility effects on its ^{1}H spectrum. These measurements lay the groundwork for *in situ*/*operando* measurements of this electrode material in device-like configurations that can inform on the behavior of protons during charge storage. We also present ^{1}H chemical shift image measurements of this material in a functioning electrochemical device that start to probe this information.

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Mark Bovee - U.S. Naval Research Laboratory
4555 Overlook Ave. SW Washington, DC, 20375 United States, Email: mark.o.bovee.civ@us.navy.mil

Structural Analysis of ^{13}C and ^{15}N Isotopically Labeled Chitin in its Natural Biological State via Solid-State NMR of *Manduca sexta* Pupal Cuticle

William A. Nese,[a] Juliana R. Burnside,[a] Sean Holmes,[b] Shubha S. Gunaga,[b] Frederic Mentink-Vigier,[b] and Terry Gullion[a]

a. West Virginia University, C. Eugene Bennett Department of Chemistry, Morgantown, WV 26506-6045
b. National High Magnetic Field Laboratory and Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32310

Chitin is ubiquitous among insects and other arthropods and is the second most abundant biopolymer. This polysaccharide, in many ways, is responsible for the success of insects since it is a major component of insect wings and exoskeletons.[1,2] The structure of chemically isolated chitin was determined via X-ray crystallography by Minke and Blackwell and later refined by Sikorski, Hori, and Wada.[2,3] Our recent solid-state NMR and DFT work found new structural conformations in isolated chitin that were not detected by previous studies, and these results will be discussed. In its natural biological state, chitin is part of a protein/chitin matrix.[1,4,5] Therefore, the question that naturally arises is what the structure of chitin in its native state is and how it differs from that when chemically isolated. To address this question, we have embarked on a study of chitin in the pupal cuticle of the tobacco hornworm (*Manduca sexta*). This study entails ^{13}C and ^{15}N isotopic enrichment of chitin to facilitate NMR methods such as REDOR, TEDOR, and homonuclear correlation experiments. A description of labeling procedures will be provided and preliminary NMR results of labeled chitin in its native state will be presented. The long-term objective is to gain a better understanding of the unique mechanical and chemical properties of chitinous components of insects.

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William Nese - West Virginia University
100 Prospect Street, Morgantown, WV 26506, United States, Email: wan00004@mix.wvu.edu

Towards Microscale NMR at 14T using Quantum Diamond Sensors

Chun Tung Cheung1, Emmeline Riendeau1, Zhiran Zhang
2, Evan Villafranca2, Ian Hammock2, Nazar Delegan2,3, F
Joseph Heremans2,3, Alexander A High 2, Joseph R
Sachleben 4 , Peter Maurer 2

1. Department of Physics, University of Chicago
2. Pritzker School of Molecular Engineering, University of Chicago
3. Material Science Division, Argonne National Laboratory
4. Biomolecular Nuclear Magnetic Resonance Facility, University of Chicago

Quantum sensors are driving the miniaturization of NMR spectroscopy toward the single-molecule level. Recent advances in quantum sensing based on Nitrogen-vacancy (NV) centers have demonstrated nm-scale NMR, mHz spectral resolution, and sub-pT/Hz sensitivity, raising hopes for NMR analysis of single biomolecules. However, early NV-NMR experiments focused on proof-of-principle demonstrations at low magnetic fields ($<3T$), which limited spectral resolution; a strong field is essential to resolve chemical shifts for molecular structure analysis.

Here, we tackle the formidable task of engineering an NV-NMR spectrometer at $14T$, converging disciplines from THz engineering, diamond material science, high-field quantum sensing, and lab-on-a-chip integration. We developed quantum control at $14T$, driving $8MHz$ Rabi oscillations of NV centers at $398GHz$ using planar metal THz metamaterials. We achieved NV-doping on (111)-cut diamond substrates using MPCVD, creating a thick layer of dense NV ensembles. Furthermore, we demonstrated sensing protocols at $14T$, showing AC magnetometry with $100nT/Hzm^3$ sensitivity. We integrated a microfluidic system with the diamond sensor chips, allowing the delivery and control of $20pL$ of analyte to the assay site.

Our $14T$ NV-NMR spectroscopy system is enabling us to resolve spectra from microscale samples with chemical specificity. This eventually allows NV-NMR to move beyond the laboratory toward real-world biochemical applications, paving the way for single-cell metabolomics, drug engineering, and beyond.

Chun Tung Cheung - University of Chicago
5640 S Ellis Ave, WERC LL250F Chicago, IL, 60637 United States, Email: ctcheung1123@gmail.com

Molecular-scale mapping of the *Pseudomonas aeruginosa* biofilm matrix

Courtney Reichhardt

Washington University in St. Louis, Department of Chemistry, St. Louis, MO 63130

Biofilms are bacterial communities encased in an extracellular matrix composed of biopolymers that are self-produced by the bacteria and, in some cases, derived from their surrounding environment. Biofilms are environmentally and industrially important and are also a major cause of persistent infections, in part due to their elevated tolerance to antimicrobial treatments. Biofilm matrices commonly include fibrillar adhesins and exopolysaccharides, both of which play key roles in biofilm formation and function. However, their structural and dynamic properties remain incompletely understood due to challenges associated with their size, heterogeneity, and limited solubility. Here, we present a multidisciplinary investigation of the *Pseudomonas aeruginosa* biofilm architecture, integrating complementary structural approaches.

Specifically, we refined the full-length structure of CdrA, a key fibrillar adhesin that promotes bacterial aggregation, by combining cryo-electron microscopy and solid-state NMR-derived restraints with computational modeling. This analysis revealed a modular architecture consisting of an extended tandem domain repeat region and an N-terminal adhesive domain with a clawlike arrangement of subdomains, providing insight into its roles in surface attachment and intercellular interactions.

Complementing this protein-focused analysis, we employed solid-state NMR spectroscopy, including experiments at high magnetic fields (900 MHz and 1.1 GHz), to characterize the composition, interactions, and dynamics of exopolysaccharides within intact biofilms. By overcoming limitations in spectral resolution while preserving native matrix organization, we identified distinct contributions of multiple exopolysaccharides to biofilm structure.

Together, these results provide an integrated view of biofilm organization. This work advances our understanding of the molecular basis of biofilm formation with implications for developing strategies to combat biofilm-associated infections, and it establishes a framework for studying other complex biological assemblies.

Courtney Reichhardt - Washington University in St. Louis
1 Brookings Dr St. Louis, MO, 63130 United States, Email: creichhardt@wustl.edu

Accelerating Protein NMR Crystallography with Machine-Learning Interatomic Potentials: ?Protonation States in the Active Site of Toho-1

Christopher G. Williams,[a] Songlin Wang,[b] Alexander F. Thome,[a] Chad M. Rienstra,[b] and Leonard J. Mueller[a]

[a] Department of Chemistry, University of California-Riverside, Riverside, CA 92521
[b] Department of Biochemistry, University of Wisconsin-Madison, Madison, WI 53706

We present the refinement of structure and protonation states of Toho-1 ß-lactamase using NMR crystallography. Enabling this approach is the nearly complete assignment of backbone and side chain chemical shifts for a microcrystalline sample of this 28 kDa protein in its inhibitor-bound form. Using only two 2D and three 3D experiments at 900 MHz, 99% of the backbone and 94% of the nonaromatic sidechains can be assigned. These experiments are complemented by high-sensitivity MAS cryoprobe measurement of the active site side chain chemical shift tensors, which for Toho are essential to the determination of protonation states.

Equally important to this approach is the development of computational models of the enzyme active site that allow for the accurate prediction of NMR spectral parameters, along with quantitative methods to assign overall confidence in the resulting structure. Here, we introduce an accelerated NMR crystallography workflow that incorporates a machine-learning interatomic potential based geometry refinement along with DFT chemical shift calculations. Incorporating MLIP accelerates the geometry optimization of the cluster models by five orders-of-magnitude (wall times from 2-6 weeks per structure optimization down to ~30 s) compared to our earlier DFT-based protocol, while retaining the high-level structural accuracy required for first-principles evaluation of NMR chemical shifts. Together, these allow for rigorous discrimination between competing protonation state models.

Together, these tools reveal a protonation-state configuration that challenges prior models and offers new mechanistic insight into ß-lactamase inhibition.

Len Mueller - University of California - Riverside
Department of Chemistry, UC Riverside Riverside, CA, 92521 United States, Email: leonard.mueller@ucr.edu

Magic-Angle Spinning Solid State NMR in a 5 mm Solution Probe via MAS-SPINDLE

Ryan Galperin,[1] Elias Herman,[1] Gemma Pham,[1] Konstantin Drallios,[1] Thomas Osborn Popp[1]

1. Oregon State University, Department of Chemistry, Corvallis, OR, 97331

Magic-angle spinning (MAS) NMR provides rich structural and dynamical information for heterogeneous solids and soft materials, but typically requires dedicated high-power instrumentation distinct from the solution state spectrometers already present in most chemistry departments and industrial laboratories. One approach to bridging this gap is to spin a rotor within the volumetric constraints of a standard NMR tube, enabling MAS experiments on solution state NMR hardware. MAS spinning in a cylindrical volume was first introduced by Zilm et al. and more recently by Wili et al. who demonstrated this concept with a device that spins a 6 mm sphere rotor up to 2.1 kHz within a 10 mm cylindrical volume.[1,2] However, the broader impact of this approach depends critically on extending the concept to 5 mm probes, the most common solution state NMR format. Here we present a 5 mm implementation of this device class, which we call an MAS-SPINDLE (MAS Solution Probe INsert Device for Line-narrowing Experiments). The MAS-SPINDLE pneumatically spins a 3.2 mm sphere rotor within a 5 mm cylinder. The spinning axis is controlled using multiple angled apertures, while magic angle adjustment is achieved by tuning relative gas flow rates across these apertures.[3] To guide device design, we developed a Python tool that predicts spinning axis angle and adjustment trajectory for arbitrary aperture geometries. Experimentally, the magic angle is set *in situ* by monitoring the ^{27}Al resonance of a single-crystal sapphire insert within the rotor cap.[4] The MAS-SPINDLE achieves spinning rates of 12 kHz or greater using compressed air (with higher rates accessible using helium), and is fully 3D printable on a benchtop stereolithographic printer (Formlabs Form 4). Ongoing work is focused on the application of low-power MAS NMR experiments to assess which measurements remain accessible on solution state and benchtop spectrometers.

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Ryan Galperin - Oregon State University
2900 SW Campus Way Corvallis, Oregon, 97331 United States, Email: galperir@oregonstate.edu

Mechanochemical Routes to Conventional and Integrative Pharmaceutical Solid Forms: Insights from PXRD and Multinuclear Solid-State NMR Spectroscopy

Peyton G. Osborn[1,2], Megan M. Joyce[3], Trisha S. Patel[1,2], Zach T. Dowdell[1,2], Sean T. Holmes[1,2], Robert W. Schurko[1,2].

[1]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL, 32306
[2]National High Magnetic Field Laboratory, Tallahassee, FL, 32310
[3]Washington and Jefferson College, Washington, PA 15301

Mechanochemistry has emerged as a powerful synthetic approach with growing impact across pharmaceuticals, materials science, and sustainable chemistry. Mechanochemical synthesis, which uses mechanical force to drive chemical reactions, can sometimes exploit synthetic pathways that are different from those found in analogous solution-based synthetic techniques. In the realm of active pharmaceutical ingredients (APIs) and nutraceuticals, mechanochemistry provides a greener and more efficient approach for synthesizing conventional, well-established solid forms, such as salts and cocrystals, and provides a powerful means for discovery of novel integrative solid forms that combine structural features of multiple simpler classes of organic crystalline solids. Examples of integrative solid forms include, among many possibilities, polyheterosalts, ionic cocrystals, and ionic solid solutions. Solid form development and screening are critical steps in drug development, as the solid form of an API can dramatically affect its physicochemical properties, such as solubility, thermal stability, and bioavailability, without negatively influencing its pharmacological activity. In this study, ball milling is used to synthesize salts and integrative solid forms, particularly ionic solid solutions, of the API dapsone. These products are characterized with powder X-ray diffraction (PXRD) and multinuclear solid-state NMR (SSNMR) spectroscopy, focusing on the nuclei ^{13}C, ^{15}N, ^{35}Cl, and ^{81}Br. We find that halogen NMR (i.e., ^{35}Cl and ^{81}Br) is very useful for the analysis of ionic solid solutions, as the patterns are significantly broadened compared to the pure salts due to the distribution of local structures caused by random substitution of halide ions throughout the lattice. Together, these results demonstrate how comprehensive structural characterization by SSNMR and PXRD provides critical insight into the architectures and compositional flexibility of solid forms of APIs obtained via mechanochemistry.

Peyton Osborn - Florida State University & National High Magnetic Field Laboratory
102 Varsity Way Tallahassee, FL, 32306 United States, Email: po23@fsu.edu

Getting the most information out of quantum noise spectroscopy

Nanako Shitara1, Pranay Venkatesh2, Tianchu Li2, Andrés Montoya-Castillo2

1. University of Colorado Boulder & University of Toronto
2. University of Colorado Boulder

Quantum sensing promises nanometer-scale, single-molecule sensitivity in the radio-frequency regime that can reveal decoherence mechanisms in quantum devices, image catalytic active sites, and even reveal single-protein structural dynamics. In particular, quantum noise spectroscopy—a form of quantum sensing that leverages pulsed NMR or EPR measurements—offers the ability to extract frequency-resolved maps of the coupling between a quantum sensor and its environment, and the potential to reconstruct nanoscale chemical distributions. However, current quantum noise spectroscopies rely on severe approximations that sacrifice accuracy and precision, and their interpretation remains bespoke. In this talk, I will discuss both signal extraction and simulation-based interpretation tools we have developed to overcome these limitations. Our signal extraction tools self-consistently extract noise spectra from commonly performed dynamical decoupling-based coherence measurements, while adopting only minimal assumptions and being resilient to measurement errors. Our methods quantify confidence intervals and sensitivity measures to identify experiments that improve spectral reconstruction. We employ our method to reconstruct the noise spectrum of a nitrogen-vacancy sensor in diamond, resolving previously undetected nuclear species at the diamond surface and revealing that previous measurements had overestimated the strength of low-frequency noise by an order of magnitude. Our method uncovers previously hidden structure with unprecedented accuracy, setting the stage for precision noise spectroscopy-based quantum metrology.

Andres Montoya Castillo - University of Colorado Boulder
1850 Folsom Street, apt 707 Boulder, CO, 80302 United States, Email: andres.montoyacastillo@colorado.edu

NMR &; MRI: More from Graph Theory, Path-Sum and Divided Difference Functions

Christian Bonhomme,1 Pierre-Louis Giscard,2

1. Laboratoire de Chimie de la Matière Condensée de Paris, Sorbonne University, Paris, France
2. Laboratoire de Mathématiques Pures et Appliquées, ULCO, Calais, France

In this presentation, we will revisit spin dynamics using graph theory and Path Sum analysis.[1] We will show that it is possible to provide exact and analytical formulas in several situations that are familiar in NMR and MRI.[2] All these results can be extended to non-hermitian matrices.

Bloch's equations will serve as a guiding thread to introduce the following concepts: (i) Differential Galois theory, (ii) Reverse-engineering, (iii) Path Sum applications including divided difference exponentials, (iv) New ways to improved numerical approximations.[3]

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Christian Bonhomme - Sorbonne University
4 place Jussieu PARIS, Ile de France, 75252 France, Email: christian.bonhomme@sorbonne-universite.fr

"Magic-angle hopping" Na-ion dynamics in a sodium antiperovskite: a distinct motional averaging mechanism of the quadrupolar interaction

Tyler Case,[1] Liangping Zhu,[2] Duhan Zhang,[2] Yifan Quan,[2] Michael A. Hope,[3] David M. Halat[1]

1. Colorado School of Mines, Golden, CO 80401, United States.
2. University of Pennsylvania, Philadelphia, PA 19104, United States.
3. University of Warwick, Coventry CV4 7AL, United Kingdom.

Antiperovskite-based solid-state fast-ion conductors are attractive systems for sensitive quadrupolar NMR measurements of ion dynamics, due to the large electric field gradient (EFG) at the cation site. In variable-temperature static ^{23}Na spectra of sodium amide borohydride antiperovskites and their deuterated analogues, we observe that rapid Na-ion motion leads to partially-averaged second-order quadrupolar powder patterns that cannot be described by simple EFG averaging; to our knowledge, these unique dynamically-averaged lineshapes have not been previously characterized. We show that these lineshapes arise from a specific Na-ion motional mechanism, namely discrete Na-ion hopping amongst three sites related by the magic angle, due to the unique cubic crystal structure of the antiperovskite phase. This mechanism nominally averages the EFG to zero, but does not eliminate the second-order quadrupolar interaction, because the orientational dependence contains fourth-rank terms. The resulting three-site lineshape is therefore distinct both from previously well-described static as well as magic-angle spinning (MAS) powder patterns. Extending the model to four- and five-site magic-angle hopping reveals a systematic progression of characteristic spectra, with the MAS-like lineshape recovered only for five-site exchange, due to the presence of fourth-rank terms. We derive empirical expressions for magic-angle hopping lineshapes and fit the variable-temperature ^{23}Na spectra of the protonated and deuterated materials, thereby extracting exchange rates and activation energies for ion motion. We also interpret this behavior as an intrinsic dynamical analogue of the magic-angle hopping experiment of Bax, Szeverenyi, and Maciel,[1] with Na-ion motion sampling three discrete orientations reminiscent of 120° hops about a magic-angle axis, although the molecular-level Na-ion dynamics (k_{ex} ~ 500 kHz) far exceed the external hopping rates accessible in prior experiments. More broadly, these results establish a practical framework for connecting MD-inspired discrete hopping models to experimental quadrupolar lineshapes in fast-ion conductors.

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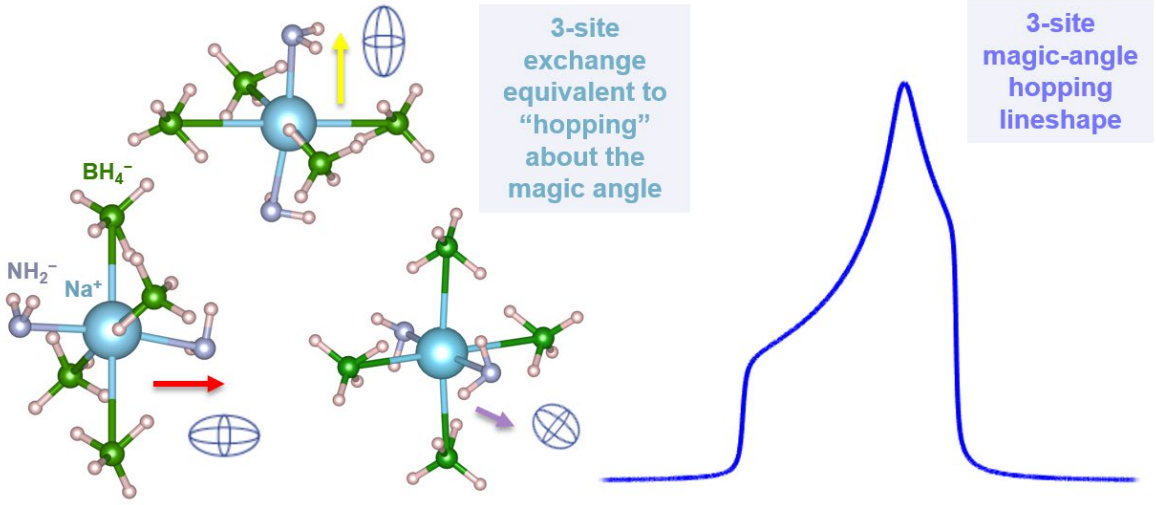

David Halat - Colorado School of Mines
164 Coolbaugh Hall Golden, CO, 80401-1887 United States, Email: david.halat@mines.edu

Structure Determination of 2D Germanane, Methyl Germanane and Methyl Germanane-Stannane Nanosheets by Nuclear Magnetic Resonance Spectroscopy

L.M. Yunusa,[1,2] Jeremy Essner,[3] Maharram Jabrayilov,[3] Abhijit Bera,[3] Bradyn C. Weaver,[1,2] Amrit Venkatesh,[4] Alexander J. Kopeny,[1] Takeshi Kobayashi,[1] Frederic A. Perras,[1,2] Rana Biswas,[1] Ivan Hung,[5] Zhehong Gan,[5] Matthew G. Panthani,[3] and Aaron J. Rossini.[1,2]

[1]Ames National Laboratory, Division of Materials Science and Engineering, Ames, Iowa, USA
[2]Department of Chemistry, Iowa State University, Ames, IA, USA
[3]Department of Chemical and Biochemical Engineering, Iowa State University, Ames, IA, USA
[4]Department of Chemistry, University of Virginia, Charlottesville, VA, USA
[5]National High Magnetic Field Laboratory, Tallahassee, FL, USA

Two-dimensional (2D) germanium-based materials have attracted considerable attention due to their tunable optical and electronic properties and potential applications in atomically thin semiconductor devices.[1] These materials are commonly synthesized by topotactic deintercalation of layered precursors such as $CaGe_2$ or SrGeSn using reagents including hydrochloric acid (HCl) or iodomethane (CH_3I).[2] However, these processes typically results in structurally disordered nanosheets with mixed surface terminations, which limits characterization by single-crystal or powder X-ray diffraction-based methods.[3] Here, we use solid–state nuclear magnetic resonance (NMR) spectroscopy, complemented by energy-dispersive X-ray spectroscopy (EDX), to probe the local structure of hydrogen terminated germanane (H–Ge), methyl terminated germanane (CH_3–Ge), and methyl terminated germanium-tin nanosheets (CH_3–GeSn). EDX analysis indicates that 13%-18% of Ge and Sn atoms are terminated by halogen species (Cl or I), depending on the deintercalation conditions. Interestingly, ~6% of methyl groups in CH_3–Ge are identified as methoxide (CH_3O-Ge), likely formed by hydrolysis of CH_3I. $^{13}CH_3$–GeSn can be easily and inexpensively prepared by using $^{13}CH_3I$ during synthesis. ^{13}C-enrichment of CH_3–GeSn enables $^{13}C^{119}Sn$ REDOR and 2D ^{13}C homonuclear correlation NMR experiments to be performed. These experiments allow carbon-tin and carbon-carbon interatomic distances to be precisely measured. Modeling of $^{13}C^{119}Sn$ REDOR curves using the INTERFACES computer program[4] confirms that CH_3–GeSn consists of a semi-ordered 2D lattice with alternating methyl terminated Ge and Sn atoms. High-field ^{73}Ge NMR further provides insight into the distribution of local electronic environments. The experimental results are in good agreement with plane-wave DFT calculations, providing experimentally validated atomistic models of these disordered materials.

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Lukman Yunusa - Iowa State University
2415 Osborn Dr 1605 Gilman Hall Ames, Iowa, 50011-3111 United States, Email: lmyunusa@iastate.edu

Probing surface terminations and lithium intercalation in $Ti_3C_2T_x$ MXene using *ex situ* NMR

Ryan J. Bragg,[1] Helena Loan,[1] and Michael A. Hope.[1]

1. University of Warwick, Department of Chemistry, Coventry, CV4 7AL, United Kingdom

MXenes are a fast-expanding class of two-dimensional transition-metal carbides, carbonitrides, and nitrides that demonstrate key properties for the development of the next-generation of supercapacitors, including high metallic conductivity, rich surface terminations and highly tuneable interlayer chemistry.[1,2] Among these materials, $Ti_3C_2T_x$ is the most prominent candidate for high-rate energy storage applications. In this work, we employ MAS ssNMR spectroscopy to perform a comprehensive characterization of the surface terminations in pristine $Ti_3C_2T_x$. We provide a thorough analysis of the termination environment, which agrees with prior assignments,[3] to establish a robust baseline for pristine $Ti_3C_2T_x$ electrodes. Following this characterization, *ex situ* NMR measurements were performed on lithiated $Ti_3C_2T_x$ electrodes to probe the local structural changes during device operation. By utilizing 2D heteronuclear correlation (HETCOR) experiments across a variety of nuclei (^{1}H, ^{7}Li, ^{13}C, ^{19}F, and $^{47/49}Ti$) on both pristine and charged electrodes, we are able to identify intercalated lithium species, demonstrating the ability of NMR to track the charging process. Furthermore, we report a charge-dependent change in the ^{1}H and ^{19}F chemical shifts correlating with -OH and -F surface terminations, respectively. These results illustrate the utility of multinuclear solid-state NMR in elucidating the complex interfacial chemistry and charge-storage mechanisms of MXene-based electrodes and lay the groundwork for future *ex situ* and potential *in situ* NMR experiments.

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Ryan Bragg - University of Warwick
University of Warwick Coventry, West Midlands, CV4 7AL United Kingdom, Email: ryan.bragg@warwick.ac.uk

NMR Crystallography of Emerging Classes of Lithium and Sodium Transition-metal Oxide and Phosphate Materials

Sarah L. Ko,[1] Jui-Cheng Hsiao,[1] Tianren Zhang,[1] Robert Krumland–Dunning,[2] Kevin J. Anderton,[1] Kent J. Griffith,[1,2]

1. University of California San Diego, Department of Chemistry, La Jolla, CA 92093
2. University of California San Diego, Program in Materials Science &; Engineering, La Jolla, CA 92093

Structural complexity—specifically, defects, dynamics, distortions, and disorder—may either underly or undermine the functional properties of an inorganic material. These critical symmetry-lowering local phenomena can be probed with an 'NMR crystallography' approach to atomic structure characterization that combines X-ray and neutron diffraction with DFT-supported solid-state NMR spectroscopy. This talk will focus on several recent examples from our laboratory including: (i) the structural and electrochemical consequences of vacancy order/disorder in intrinsically defective anti-NASICON niobium phosphates[1]; (ii) new lithium-rich "layered" structures, Li_3MO_4 (*M* = Nb, Ta) synthesized via instantaneous ion exchange in a molten salt flux[2]; and (iii) point defect chemistry and defect tolerance in $NaNb_7O_{18}$ and $NaNb_{13}O_{33}$ framework structures with tunnel-blocking Na^+ ions[3].

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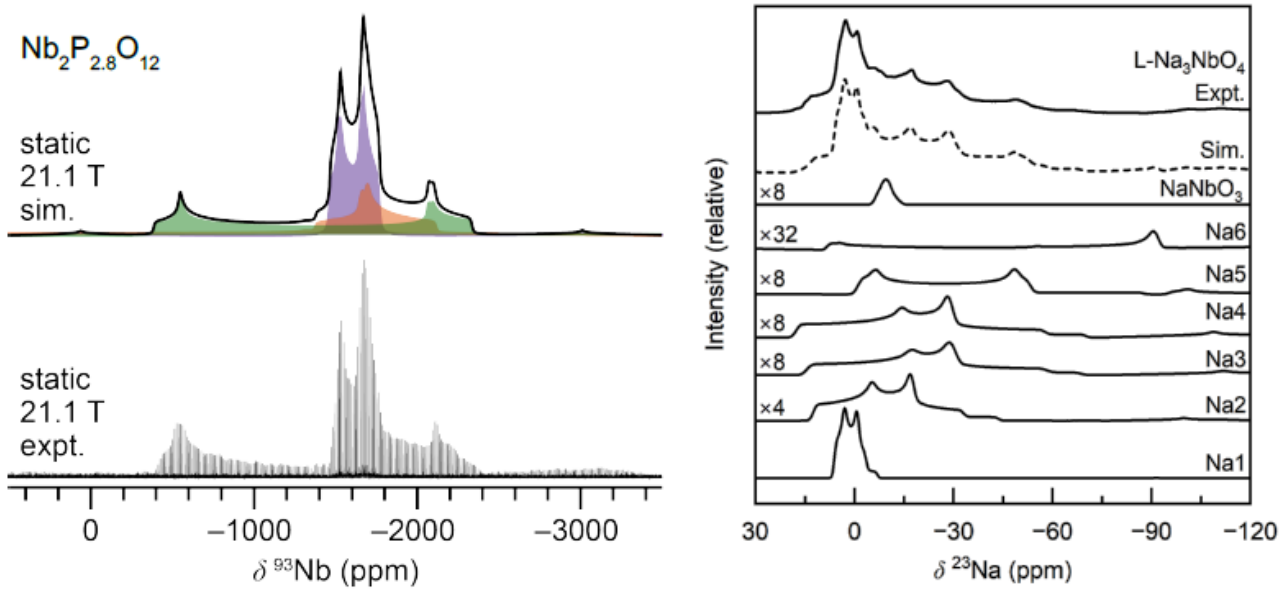

Kent Griffith - University of California San Diego
9500 Gilman Drive La Jolla, CA, 92093 United States, Email: k3griffith@ucsd.edu

Solid-State NMR Strategies for Probing Rare Earth Structure and Dynamics

Brennan J. Walder, Tanya Prozorov, Carl H. Fleischer III, Frédéric A. Perras

Ames National Laboratory, Chemical and Biological Sciences Division, Ames, Iowa 50011

Every NMR active isotope of the rare-earth elements (Sc, Y, and the lanthanoids) is either quadrupolar, low-?, engages in hyperfine interactions, or some combination of these. Because of these properties, solid-state NMR is rarely applied to structurally complex rare-earth systems. Here, I present solid-state NMR approaches for probing scandium and lanthanum environments in clays and in extraction media relevant to rare-earth separation processes. Reverse CP experiments tailored to quadrupolar nuclei at 50 kHz MAS are effective for detecting ^{1}H environments near ^{45}Sc in rare-earth adsorbing clays. Exchange experiments reveal nonuniform rare-earth distributions between the clay and impurity phases and highlight that hydration enhances the dynamics of the metal coordination environment. I then turn from clay adsorption systems to liquid extraction systems and show how DNP enhanced solid-state ^{139}La NMR enables structural characterization of lanthanum coordination complexes in a vitrified ethylene glycol:maleic acid eutectic solution. Quantitative La-ligand atom distances in the glassy extraction medium are obtained using ^{13}C^{139}La RESPDOR and TEDOR-like ^{1}H^{139}La dipolar recoupling experiments. Molecular dynamics and electronic structure calculations, constrained by the NMR observables, yield atomistic models of the La coordination complexes. These models clarify the structure and dynamics of rare-earth species in both clay and extraction environments relevant to critical mineral separations.

Brennan Walder - Ames National Laboratory
340B Spedding Hall, 2416 Pammel Dr Ames, IA, 50011 United States, Email: bwalder@ameslab.gov

Multi-Nuclear Solid State NMR Studies of Structure-Property Relationships in Glass, with Applications Ranging from Nuclear Waste Storage to High-Performance Optics

U. Werner-Zwanziger[1], P. A. Bingham[2], M. Onaru[2], J. Zwanziger[1]

1. Department of Chemistry, Dalhousie University, Halifax, NS B3H 4R3 Canada
2. Materials and Engineering Research Institute, College of Business, Technology and Engineering, Sheffield Hallam University, City Campus, Sheffield, S1 1WB, UK

The local structure around glass forming and glass modifying groups influences macroscopic glass properties, among them optical behaviour, crystallization and mechanical response. Here we use a multi-nuclear NMR approach to gain insights into the structure-property relationships in a variety of glasses, ranging from nuclear waste model systems to zero-stress optic glasses. For nuclear waste model glasses we combine the structural information obtained from ^{31}P, ^{11}B, ^{29}Si and ^{23}Na NMR with detailed oxygen balance calculations and thereby reveal the driving force behind the onset of crystallization[1]. For tellurite glasses we show how from the study of a series of crystalline compounds correlating the chemical isotropic and anistropic shifts in relation to bond angles and coordination numbers, we can gain insight into the glass structure[2,3]. We combine these experimental results with DFT calculations to form a comprehensive picture of the bonding[4]. Using detailed studies of ^{207}Pb NMR in glasses combined with recent DFT calculations, we obtain insight into the unique optical behaviour bestowed by the lead bonding, which is exploited to create zero-stress optic glasses. And finally, we show how the Czjzek distributions of ^{139}La in lanthanide glasses is important to understand the bonding in lanthanum-containing glasses[5].

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Ulrike Werner-Zwanziger - Dalhousie University
6245 Castine Way, PO BOX 15000 Halifax, NS, B3H 4R2 Canada, Email: Ulli.Zwanziger@Dal.ca

Structural Defects in Glass: are traditional models being called into question?

Pierre Florian,(1) Daniel R. Neuville ,(2) Thibault Charpentier,(3) Franck Fayon(1)

(1) CEMHTI UPR3079 CNRS, Univ. Orle´ans, F-45071 Orle´ans, France
(2) IPGP UMR7154 CNRS, Ge´omate´riaux, Paris Sorbonne Cite´ , 75005 Paris, Franc
(3) NIMBE, CEA, CNRS, Universite´ Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette Cedex, France

In glass science, the prevailing view based on arguments regarding charge compensation largely determines how scientists think about the structure of glass. This approach not only drives the design of new materials, but also informs our understanding of macroscopic properties in the molten state, such as viscosity, since glasses are considered to be 'frozen liquids'. In aluminosilicate systems, the 'common wisdom' is that the ratio of 'network modifiers' (e.g. alkali or alkaline earth cations) to aluminium controls the network topology. However, it has been demonstrated that defects can be present at low levels. For example, some non-bridging oxygen (NBO) can form and disrupt network connectivity unexpectedly, and high-coordinated aluminium units can change the topology. In this regard, nuclear magnetic resonance has played a pivotal role in examining both the glassy state[1] and high-temperature melts.[2]
Here, we use ^{27}Al and ^{17}O NMR spectroscopy to explore the SrO-Al2O3-SiO2 phase diagram, examining both glasses and melts (up to 1900 °C). We demonstrate the presence of high-coordinated AlO5 aluminium species in regions where they are not expected. We also observe NBO on AlO4 units, which are lost during cooling from the melt when the concentration of SiO2 is high. Newly developed MAS cryoprobe at high-field (20.0 T) provide enough sensitivity increase such that ^{17}O NMR is now possible at natural abundance in those compositions. This allowed us to explore, without ^{17}O labelling, the supposedly fully connected network of compositions along the ‘charge compensation’ line of the SrO-Al2O3-SiO2 phase diagram. We extract the experimental content of 'forbidden' network-breaking NBO as a function of composition, comparing it to molecular dynamics simulations.[3] We also explore how cooling rate affects the number of NBOs, and discuss the potential of oxygen-17 ssNMR for identifying tri-coordinated oxygen sites.

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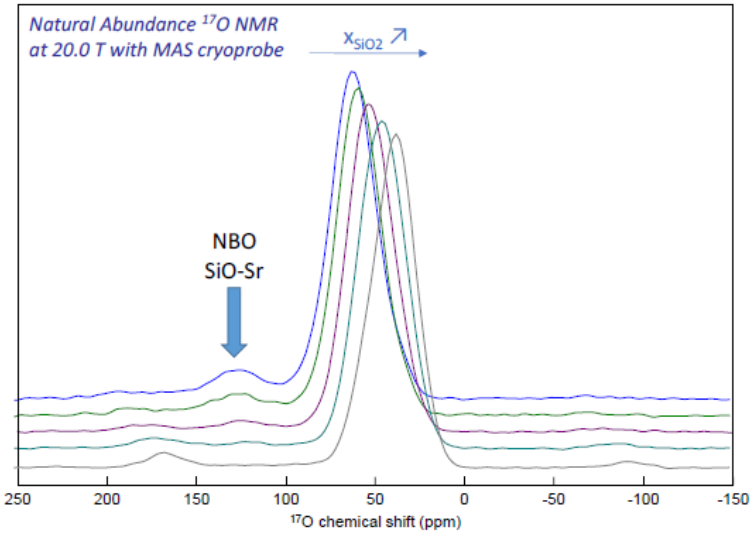

Pierre Florian - CEMHTI-CNRS
1D Av. Recherche Scientifique Orleans, Centre Val de Loir, 45071 France, Email: pierre.florian@cnrs-orleans.fr

Inverse Methods for Nuclear Magnetic Resonance of Non-Crystalline Materials

Philip J. Grandinetti

Department of Chemistry, The Ohio State University, Columbus, Ohio, USA

The atomic-scale structure of non-crystalline materials—central to technologies from chemically tempered glass in consumer electronics to bioactive implants—remains one of the outstanding challenges in materials science, with structural disorder governing key properties such as ionic transport, chemical durability, and mechanical strength. Conventional structure-forward approaches rely on molecular dynamics simulations subsequently validated against NMR spectra, but they are inherently limited by force-field accuracy and system size, often reflecting the potential model more than the experimental data. A fundamentally different strategy—spectrum-inversion—extracts quantitative probability distributions of nuclear interaction tensor parameters directly from experimental spectra, then maps those distributions onto local structural features through quantum-chemical relationships. I will describe our spectrum-inverse framework built around a Smooth-LASSO regularization algorithm that robustly solves the ill-posed Fredholm inversion of two-dimensional isotropic/anisotropic correlation NMR spectra into trivariate distributions of nuclear shielding tensor parameters. Applied to ^{29}Si 2D NMR spectra of network-modified silicate glasses, this approach yields quantitative, model-free distributions that resolve Q^n speciation and reveal how modifier cation identity and content influence Si–O bond length and network connectivity distributions—structural detail completely invisible in conventional 1D MAS spectra. I then present results for ^{31}P NMR of potassium and sodium phosphoaluminosilicate glasses, where inverting 2D Magic-Angle Flipping spectra reveals distinct Q^n_P environments distinguished by their second-coordination sphere, providing new insight into how phosphorus depolymerizes the aluminosilicate network and accelerates ion exchange during chemical tempering. Quantum-chemical calculations on phosphorus-centered clusters validate these tensor-to-structure assignments. These methods are implemented in the open-source Python packages MRSimulator and MRInversion.[1]

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Philip Grandinetti - Ohio State University
100 West 18th Avenue Columbus, OH, 43210 United States, Email: grandinetti.1@osu.edu

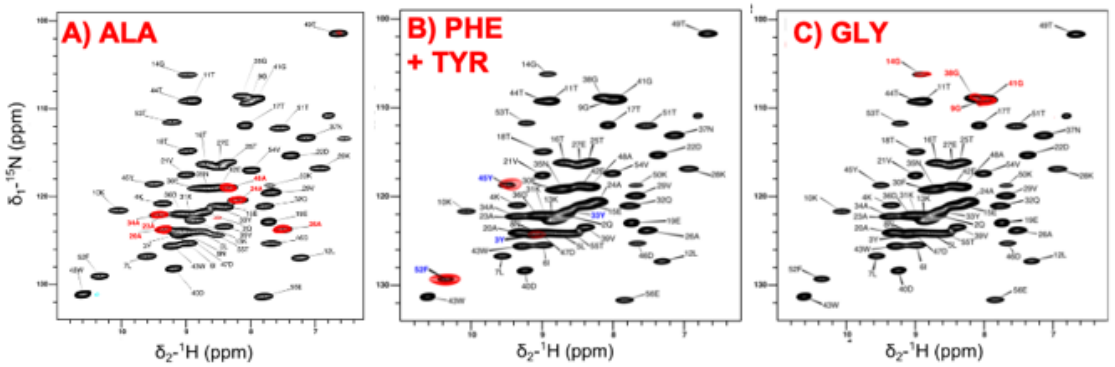
Chemical Shift Based Amino Acid-Type Spectral Editing for Backbone Atoms and Residue Centric Distance Restraint Mapping in Fast Magic Angle Spinning U-[^{13}C,^{15}N] Proteins

Vipin Agarwal, Mopidevi Mohana Venkata Subbarao, Sahil Ahlawat and Sreejith Raran-Kurussi

Tata Institute of Fundamental Research Hyderabad, Sy. No. 36/P, Gopanpally, Hyderabad, India, 500 046, Email: vipin@tifrh.res.in

Unambiguous assignment of amino acid types and resonances remains a central challenge in protein structure analysis by solid-state nuclear magnetic resonance (NMR), particularly as protein size and complexity increase, leading to severe spectral overlap and assignment ambiguities. Conventional strategies to mitigate spectral crowding generally involve elaborate isotope labeling protocols, such as stereo-array isotope labeling, methyl-selective labeling, or 2-glycerol labelling or acquisition of higher-dimensional (3/4/5-D) spectra, both of which significantly increase experimental demands. Herein, we present rapid and versatile spectral editing methods applicable to U-^{13}C,^{15}N -labelled proteins that enable amino acid type-selective detection without the need for specialized labelling schemes. Routine ^{1}H detected 2D ^{1}H-^{15}N and ^{1}H^{a}-^{13}C^{a} CP-HSQC (cross-polarization heteronuclear single quantum coherence) spectra of backbone atoms are recorded for either an individual residue type (Ala, Thr, Gly etc) or as a group of residues (e.g. residues containing methyl groups or aromatic side chains) in the fast MAS regime. These filters can also be combined with unidirectional polarization transfer approaches to identify backbone atom peaks of sequentially connected next neighbour residue. The spectral editing methods when combined with selective recoupling techniques (such as BASS-SD, SERP etc.) enable mapping of structural restraints involving side chains of specific residue-type. As an example, distance restraints involving the sidechains of the elusive aromatic residues will be highlighted. Supported by the Department of Atomic Energy, Government of India, under Project Identification RTI 4007.
Figure: shows overlay of 2D ^{1}H-^{15}N CP-HSQC spectra of U-[^{13}C,^{15}N] labelled GB1 spectra (black) with 2D ^{1}H-^{15}N CP-HSQC spectra for specific amino acids (red) acquired on the same sample at MAS frequency ~95kHz and Static field of 700 MHz. As an example, three amino acid specific spectra (red) are shown A) ALA, B) Combined PHE and TYR and C) GLY.

Figure: shows overlay of 2D ^{1}H-^{15}N CP-HSQC spectra of U-[^{13}C,^{15}N] labelled GB1 spectra (black) with 2D ^{1}H-^{15}N CP-HSQC spectra for specific amino acids (red) acquired on the same sample at MAS frequency ~95kHz and Static field of 700 MHz. As an example, three amino acid specific spectra (red) are shown A) ALA, B) Combined PHE and TYR and C) GLY.



Vipin Agarwal - TATA Institute of Fundamental Research
Sy. No. 36/P, Gopanpally, Ranga Reddy District RANGAREDDY, Telangana, Hyderabad India, Email: vipin@tifrh.res.in

Repulsion-Driven Superionic Conductivity in $La_2Mo_2O_9$ monitored by DFT-assisted NMR spectroscopy

Adriana Bocchini,[1,2] Abdulkadir O. Biffo,[3] Theodosios Famprikis,[4] Klaus Lips,[5] Wolf Gero Schmidt,[1] Pedro B. Groszewicz,[3,5] Uwe Gerstmann.[1]

1. Universität Paderborn, Department of Physics, 33095 Paderborn, Germany
2. Universität Paderborn, Institute for Photonic Quantum Systems (PhoQS), 33095 Paderborn, Germany
3. Delft University of Technology, Mekelweg 15, Delft, The Netherlands
4. University of Oxford, Department of Chemistry, OX1 3QR Oxford, United Kingdom
5. Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, Berlin, Germany

The transition towards renewable forms of energy is, among other factors, influenced by the high operating temperatures of commercial solid oxide cells. In this context, $La_2Mo_2O_9$ (LAMOX), is considered a promising candidate for a new generation of solid electrolytes. Its cubic phase provides high ionic conductivity already at intermediate temperatures (600 °C). However, the ionic migration mechanism remains elusive, owing to the very large unit cell and the significant structural disorder among oxygen sites in this material. In this work, ^{17}O NMR spectroscopy is systematically employed to investigate the local oxygen environments and their role in oxygen-ion conduction: While DFT calculations unambiguously attribute five different ^{17}O coordination environments to the ^{17}O NMR spectrum, temperature-dependent LASERMAS ^{17}O NMR rules out the participation of some O^{2-} species in the superionic conducting phase. Other than previously assumed, strongly La-coordinated O atoms do not take part in the ionic migration but can be rather considered part of the rigid lattice composed by La^{3+} and Mo^{6+} cations. These oxygen species are therefore crucial for the superionic conduction, since they repulsively interact with mobile O^{2-} species guiding them to neighboring MoO_x polyhedra. Furthermore, the presence of a so-far unresolved interstitial enables the activation of a cascade of inter-polyhedral oxide-ion jumps and thus long-range ionic conduction. We expect our DFT+NMR finding of repulsion-driven ion conductivity to be instrumental for the design of new superionic conductors and hence more efficient devices.

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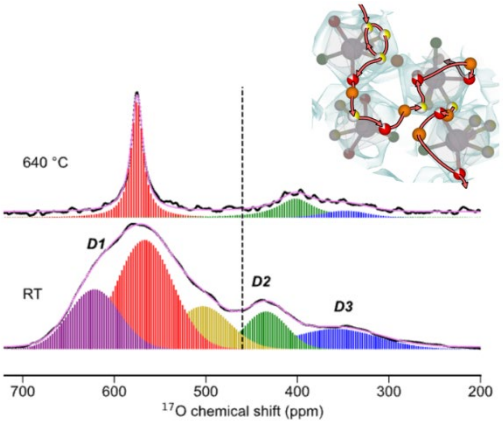

Adriana Bocchini - Paderborn University
Warburger Str. 100 Paderborn, NRW, 33098 Germany, Email: adriana.bocchini@upb.de

Probing the local environment of quadrupolar isotopes in materials using ultra-high-field NMR and advanced pulse sequences

Yury Kolyagin[1,2], Tamali Nag[1], Lama Hamdouna[1], Céline Moussa[1], Andrew G. M. Rankin[3], Julien Trébosc[3], Laurent Delevoye[1], Frédérique Pourpoint[4], Jean-Paul Amoureux[1], Olivier Lafon[1]

[1]Univ. Lille, CNRS, Centrale Lille, UCCS, Lille, France
[2]National Institute of Chemistry, Ljubljana, Slovenia
[3]Univ. Lille, CNRS, Centrale Lille, IMEC, Lille, France
[4]IUF, Paris, France

Solid-state NMR spectroscopy can provide unique insights into the atomic-level structure of defects in materials, which have a major influence on their properties. Nevertheless, major limitations of this technique remain. For instance, its lack of resolution and sensitivity for quadrupolar nuclei with spin $I = 1$, which represent over 74% of NMR-active isotopes and are the only NMR-active isotopes to observe the majority of chemical elements. [1]. We show how recent instrumental and methodological developments open new avenues for the observation of these quadrupolar isotopes. In particular, we have leveraged the gain in resolution provided by our 1.2 GHz NMR spectrometer (B_0 = 28.2 T) to obtain novel insights into the local environments of quadrupolar nuclei, such as ^{17}O, ^{33}S, ^{27}Al, ^{23}Na, ^{63}Cu, ^{71}Ga or ^{67}Zn, in solids. This approach has been applied to shed light on the mechanosynthesis of organometallic complexes and Na^+ conducting sulfur-based materials, [2] and to characterize interfaces in ZnS@ZnO shell-core heterostructures [3]. We have also developed advanced NMR experiments to probe proximities in solids between quadrupolar nuclei and protons, and between two distinct quadrupolar isotopes [4,5].

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Olivier Lafon - Univ. Lille
Avenue Mendeleiev Lille, Hauts de France, 59000 France, Email: olivier.lafon@univ-lille.fr

Interpreting chemical shielding tensors: a well-posed approach through real-space analysis

Josef W. Zwanziger

Department of Chemistry, Dalhousie University, Halifax B3H 4R2, Nova Scotia, Canada

The chemical shielding tensor is the primary object of interest in most NMR studies of solids, both computational and experimental. Using the shielding as a probe of bonding raises several challenges, if more detail is desired than a simple match between calculated values and a set of known test compounds. In particular, there are two types of gauge invariance issues that must be addressed. First, there is the well known gauge of the magnetic vector potential, which can be accommodated in several ways to yield a gauge invariant shielding, although even here ambiguity remains in making artificial separation between contributions, say paramagnetic and diamagnetic terms. Secondly, and probably less widely appreciated, is that the total shielding should be invariant to the choice of orbital decomposition in the interpretation scheme. Such invariance is likely impossible to impose rigorously.

Here we explore an alternative approach, which is well-posed and manifestly gauge invariant (in both senses discussed above), by focusing on the chemical shielding as represented as a density in real space. Our work follows on the pioneering studies of Jameson and Buckingham.[1] We discuss first the source of the gauge issues mentioned above, and demonstrate how and where in interpretations they lead to ambiguities. Then we show how a real-space representation is obtained in a solid-state calculation, and how it may be visualized and analysed, without initial orbital decomposition. Examples will be shown on atoms, molecules, and extended solids.

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Josef Zwanziger - Dalhousie University
PO Box 15000 Halifax, NS, B3H 4R2 Canada, Email: jzwanzig@dal.ca

^{1}H led NMR Structure Determination in Molecular Solids

Jacob B. Holmes[1,2], Daria Torodii[1], Ruben Rodriguez-Madrid[1], James J. Kimball[1], Lyndon Emsley[1,2]

[1] Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland
[2] National Centre for Computational Design and Discovery of Novel Materials MARVEL, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.

Rich chemical understanding is critically important to understanding function in all chemical systems. Here, we show how the determination of complete three-dimensional structures can be improved and accelerated for materials at natural isotopic abundance using new experimental methods with >100 kHz MAS, machine-learned chemical shift predictions, and rapid assignment methods, to validate structures within hours. We highlight these advances with the first demonstration of ^{1}H-^{1}H J-couplings in solids, structure validation using only ^{1}H-detected methods, the improvement of ShiftML to DFT accuracy, and the use of probabilistic methods for chemical shift assignment. The methods are combined to determine complete atomic-level structures of disordered molecular solids.

Jacob Holmes - EPFL
Avenue François-Alphonse Forel Lausanne, Vaud, 1015 Switzerland, Email: jacob.holmes@epfl.ch

High-Field MAS DNP toward In-Situ Amyloid Structural Biology

Yoh Matsuki

Institute for Protein Research, The University of Osaka

We have been developing methods and instruments for closed-cycle helium MAS-based high-filed DNP NMR[1,2,3,4]. Not only the sensitivity gain, our focus is on target-selective DNP using unpurified mixture samples. To this end, we have recently developed methods for nano-space selective observation[5] and background signal suppression[6]. We also discovered nano-diamond as a promising polarizing agent that remains efficient under strongly reducing conditions such as in cytosol, being viable for DNP at high-field (16.4 T) and under the sample spinning condition[7]. With these novel bases, we are after in-cell amyloid structural biology and in-mouse brain MRI that visualizes polymorph-dependent synaptic transmission. In the presentation, I will discuss the latest results on such methods, instrument and applications.

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Yoh Matsuki - The University of Osaka
3-2 Yamadaoka Suita, Osaka, 565-0871 Japan, Email: yoh@protein.osaka-u.ac.jp

Unraveling Interactions in Heterogeneous Catalysts using Fast MAS Solid-State NMR and EPR Spectroscopy

Dulani K. Kumarasinghe,[1] Adam Elbash,[1] Veronica S. M. Curran,[1] James W. Harris,[2] Tibor Szilvási,[2] Charles W. Machan,[1] Sen Zhang,[1] Amrit Venkatesh[1]

1. Department of Chemistry, University of Virginia, Charlottesville, VA 22904
2. Department of Chemical and Biological Engineering, University of Alabama, Tuscaloosa, AL 35487

^{19}F solid-state NMR spectroscopy is a sensitive probe of local chemical environments owing to its high Larmor frequency, 100% natural abundance, and wide chemical shift range. However, spectral resolution is often limited by large anisotropic interactions and line broadening, particularly in heterogeneous and paramagnetic catalytic systems. Here, we demonstrate that fast magic angle spinning (MAS) combined with ^{1}H-^{19}F double-resonance methods enables high-resolution ^{19}F solid-state NMR of complex catalytic materials, including systems containing paramagnetic centers. We first examine perfluorinated zinc phthalocyanine (0.05 wt%) encapsulated within Faujasite zeolites that are efficient gas-phase CO oxidation catalysts. Fast MAS reveals distinct ^{19}F chemical shifts relative to surface-deposited species, consistent with confinement-induced perturbations. Density functional theory (DFT) calculations indicate deviations from molecular planarity imposed by pore constraints. Investigations of these systems using dynamic nuclear polarization to enhance sensitivity at low loadings are currently underway. Next, we investigate fluorinated ionomers confined within mesoporous inorganic nanomaterials, where interactions with surface metal oxide nanoclusters induce paramagnetic broadening and rapid longitudinal relaxation. Fast MAS partially mitigates these effects, enabling characterization of ionomer–support interactions. Finally, X-band continuous wave EPR spectroscopy is used to probe paramagnetic Fe(III) catalysts immobilized on polymer blend supports for electrocatalytic CO_2 reduction and oxygen reduction reactions. Complementary solid-state NMR measurements provide insight into polymer–catalyst interactions. Collectively, these results demonstrate that fast MAS solid-state NMR, in conjunction with EPR, enables the characterization of low-abundance fluorinated species, resolves subtle structural perturbations, and provides molecular-level insight into confinement, interfacial interactions, and paramagnetic effects in heterogeneous catalytic materials.

Amrit Venkatesh - University of Virginia
409 McCormick Road, P.O. Box 400319 Charlottesville, VA, 22904 United States, Email: amrit.venkatesh@virginia.edu

400 **SSNMR Poster Session**

HTRA1 Forms Multimeric Assemblies with TDP-43: A Solid-State NMR Study

Arshad Abdulvahid[1], Nitin K. Pandey[1], Gincy George[1], Ralf Langen[1], Angar B. Siemer[1]

1. Department of Physiology and Neuroscience, Zilkha Neurogenetic Institute, Keck School of Medicine, University of Southern California, Los Angeles, California 90033, United States

In this poster, we present solid-state NMR data acquired at 1.1 GHz on HTRA1 (36 kDa), which forms a non-crystalline oligomeric chaperone complex. High temperature requirement A1 (HTRA1) is a widely expressed human serine protease that regulates numerous physiological processes through its proteolytic activity. In addition to its protease function, HTRA1 has been shown to act as a chaperone by inhibiting amyloid aggregation; however, the precise mechanisms underlying these activities remain elusive. Here, we investigate the interaction between TAR DNA-binding protein 43 (TDP-43) and HTRA1. In the presence of TDP-43, HTRA1 forms complex multimeric assemblies. Solid-state NMR measurements of a protease-inactive form of HTRA1 reveal that it adopts highly ordered assemblies. These findings provide new insights into the role of HTRA1 in modulating TDP-43 aggregation.

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Arshad Abdulvahid - University of Southern California
1501 San Pablo Street Los Angeles, California, 90033 United States, Email: abdulvah@usc.edu

^{23}Na NMR Studies of Amorphous Chlorides for Solid-State Na-ion Batteries

Kevin J. Anderton,[1] Feng Li,[2] Zheng Chen,[2] Kent J. Griffith[1]

University of California, San Diego, Department of Chemistry and Biochemistry, La Jolla, CA 92093University of California, San Diego, Aiiso Yufeng Li Family Department of Chemical and Nano Engineering, La Jolla, CA 92093

Chloride-based solid electrolytes have recently emerged as promising candidates for applications in solid-state sodium-ion batteries. Improved ionic conductivity and battery performance relative to pure, bulk phases can be obtained in this family of materials by altering the sodium stoichiometry and anionic composition. While partially substituted materials produced by high-energy mechanical milling can exhibit liquid-like ionic conductivity, the resulting amorphization hinders understanding of the composition and structure of these phases, as well as the mechanisms responsible for improvements in ionic conductivity. Here, solid-state NMR measurements of amorphous substituted derivatives of $NaTaCl_6$ and Na_2ZrCl_6 are employed to investigate the chemical transformations that occur during synthesis, the composition of the high-conductivity products, and their Na-ion dynamics.

Kevin Anderton - University of California, San Diego
9500 Gilman Drive La Jolla, California, 92093 United States, Email: kanderton@ucsd.edu

A ^{1}H NMR Investigation of a Birnessite-like MnO*x* Electrode Material

Mark O. Bovee,[1] Christopher A. Klug,[1] Eliana S. Dolven-Miller,[2] Ryan H. DeBlock,[1] Zoey Warecki,[3] Zachary G. Neale,[1] Debra R. Rolison,[1] and Jeffrey W. Long[1]

1. Chemistry Division, U.S. Naval Research Laboratory, Washington, DC, USA
2. Science and Engineering Apprenticeship Program, U.S. Naval Research Laboratory, Washington, DC, USA
3. Materials Science and Technology Division, U.S. Naval Research Laboratory, Washington, DC, USA

Lithium-ion battery technology dominates the rechargeable energy-storage device market;[1] however, flammability[2] and supply chain[3] concerns motivate the search for complementary alternatives.Aqueous electrochemical devices that incorporate alkali salt electrolytes and manganese oxide (MnO*x*) electrode materials can address these issues, but both the electrolyte's cations and protons can insert into these devices' MnO*x* electrode during charge storage. Because protons generally have higher solid-state mobilities, in some cases it may be advantageous to prioritize their involvement when optimizing electrochemical performance.[4] This underscores the importance of understanding how protons are incorporated into these materials and their behavior during the energy storage process.Herein, we utilize static ^{1}H NMR spectroscopy to investigate the structural environments available to protons in a birnessite-like manganese oxide electrode formed through the electroless deposition of MnO*x* onto carbon nanofoam paper (MnO*x*@CNFP). Its ^{1}H spectrum contains two features attributed to water molecules at different distances away from paramagnetic Mn ions in the material's octahedral MnO_6 layers. Additionally, selective inversion measurements reveal chemical exchange occurs between these environments in a multistep process, and measurements of MnO*x*@CNFP at different orientations with respect to B_0 demonstrate the influence of bulk magnetic susceptibility effects on its ^{1}H spectrum. These measurements lay the groundwork for *in situ*/*operando* measurements of this electrode material in device-like configurations that can inform on the behavior of protons during charge storage. We also present ^{1}H chemical shift image measurements of this material in a functioning electrochemical device that start to probe this information.

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Mark Bovee - U.S. Naval Research Laboratory
4555 Overlook Ave. SW Washington, DC, 20375 United States, Email: mark.o.bovee.civ@us.navy.mil

Rethinking isotopic substitution for NMR studies: Impacts of deuteration on sodium dynamics in sodium amide borohydride

Tyler Case,[1] Liangping Zhu,[2] Duhan Zhang,[2] Kwangnam Kim,[3] David M. Halat,[1] Yifan Quan[2]

Colorado School of Mines, Department of Chemistry, Golden, CO 80401University of Pennsylvania, Department of Chemistry, Philadelphia, PA 19104Lawrence Livermore National Laboratory, Livermore, CA 94550

NMR spectroscopists rely on deuteration to study dynamics in a variety of systems including proteins and ion conductors, claiming that isotopic substitution has no impact on the dynamics of the system. The ubiquity of this technique is such that its effect is rarely tested directly in a proton-rich system. Misunderstanding the impact of deuteration on dyamics impacts a large body of literature in chemistry, biological sciences, and materials science. Here we report ^{23}Na solid-state NMR spin-lattice relaxometry data that challenges this assumption, comparing sodium dynamics in sodium amide borohydride/borodeuteride, a promising antiperovskite sodium-ion conductor. Conveniently, this system has a near-ambient orthorhombic-cubic phase transition allowing access to the dynamics of two distinct phases from -15 °C to 60 °C. We find that the sodium ion hopping rate is depressed in the deuterated lattice across both phases. By fitting the data using the Bloembergen-Purcell-Pound theory to extract activation energy, we find that the activation energy in the deuterated sample is ~40 meV lower, also across both phases. The Meyer-Neldel relationship implies that activation energy and the Arrhenius prefactor, which encodes the attempt frequency, shift together in the same direction. We explore this relationship to explain our observations and apply them to new isotopologues in this family. This 2x2 isotopologue study of $Na_2(NH_2/ND_2)(BH_4/BD_4)$ is underway to resolve the anion sublattice contributions to the observed changes in dynamics. To this end we use ^{11}B, ^{14}N, ^{2}H, and ^{23}Na relaxometry and variable temperature impedance spectroscopy. We will discuss what these effects mean for the interpretation of isotopic substitution NMR studies in the context of these ion conductors and provide some context for careful consideration of the impacts of deuteration in similar systems. Additionally, deuteration of the azanide anion in these materials has never been reported and so is presented here for the first time.

Tyler Case - Colorado School of Mines
1500 Illinois St. Golden, Colorado, 80401 United States, Email: tyler_case@mines.edu

Probing the Structures and Dynamics of Cobaltocenium Salts via Ultra-Wideline ^{59}Co Solid-State NMR

Dominic C. Chantra,[1,2] Sara Termos,[1,2] Sean T. Holmes,[2] Robert W. Schurko.[1,2]

1. Florida State University, Department of Chemistry &; Biochemistry, Tallahassee FL 32306
2. National High Magnetic Field Laboratory, Tallahassee FL 32310

Solid-state NMR (SSNMR) is a powerful tool for probing molecular-level structure and dynamics; however, many nuclides remain a challenge due to low receptivity, including unfavorable relaxation characteristics and/or large anisotropic interactions. For half-integer quadrupolar nuclei such as ^{59}Co (I = 7/2), the second-order quadrupolar interaction and chemical shift anisotropy can yield central transition (CT, +1/2 ?? –1/2) ultra-wideline (UW) powder patterns that may be several MHz in breadth. In such cases, the use of frequency-swept pulses such as *wideband uniform-rate smooth-truncation* (WURST) pulses,[1] in tandem with signal-to-noise enhancing *Carr-Purcell-Meiboom-Gill* (CPMG) sequences,[2] enable efficient acquisition of uniform CT patterns under static conditions.[3] This study addresses the challenges of acquiring ^{59}Co UW SSNMR spectra of the cobaltocenium complexes $[Cp_2Co][PF_6]$ and $[Cp^*_2Co][PF_6]$ ($Cp = C_5H_5$; $Cp^* = C_5Me_5$). Spectra were acquired at 18.8 T and 14.1 T, with temperatures ranging from 120 to 300 K using the WURST-CPMG sequence and variable-offset cumulative spectroscopy, allowing for detection of these patterns with breadths >2.5 MHz in under one hour. From these data, the chemical shift and electric field gradient tensors were determined and found to be in good agreement with those predicted by DFT calculations. NLMO analysis was also employed to understand the orbital contributions to these tensors. Additionally, temperature-dependent T_2 measurements are used to shed light on the solid-state dynamics in these samples. These new findings, together with previous work on metallocenes,[4] provide valuable insights into their structure, bonding, and dynamics, which may guide the rational design of new metallocenes with tunable bonding characteristics. Supported by DE-SC0022310.

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Dominic Chantra - Florida State University
1653 Atkamire Dr, Unit 2 Tallahassee, FL, 32304 United States, Email: dcc24@fsu.edu

Surface-Only NMR of Calcium Silicate Hydrate: Advancing Surface-Selective Methods to the Atomic-Level Surface Structure Of Cements

X. Ray Cowen,[1,2] Tristan Georges,[1] Karen Scrivener,[2] Lyndon Emsley[1]

1. École Polytechnique Fédérale de Lausanne, Laboratory of Magnetic Resonance, Institut des Sciences et Ingéniere Chemiques, 1015 Lausanne, Switzerland
2. École Polytechnique Fédérale de Lausanne, Laboratory of Construction Materials, Institut des Matériaux, 1015 Lausanne, Switzerland

Demand for cement, currently over 4 billion tonnes annually, is projected to continue to grow in the coming decades, driving the need for new, sustainable cements. The development of such cements necessitates a complete understanding of the structure of the main binding phase, calcium silicate hydrate (CSH). Nuclear magnetic resonance (NMR) spectroscopy has proven to be a powerful tool in the atomic-level study of CSH; from its first use in the 1980s,[1] to the observation of the later stages of the hydration reaction[2] or the determination of the bulk structure of CSH.[3] However, direct experimental probes of the surface structure remain elusive. The extremely thin nature of CSH (~5 nm), and the ubiquity of hydrogen atoms throughout the structure, makes the application of even traditional surface-selective NMR techniques impossible. Here, for the first time, we experimentally differentiate the surface structure from the bulk using new surface-only NMR methods. Through the combination of dynamic nuclear polarization (DNP) methods with selective deuteration, we isolate NMR signals from silicate units originating exclusively at the surface of CSH, thus allowing for characterization of the surface structure. This breakthrough allows for analysis of the surface of CSH and its variants to uncover connections between atomic structure and macro-scale properties.

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Ray Cowen - EPFL
Av. F.-A. Forel 2 Lausanne, VD, 1015 Switzerland, Email: ray.cowen@epfl.ch

Utilizing 3D-Printing and Electroplating to Develop Solid State NMR Probe Components

Jeffrey J. Dykstra[1], Annie V. McAllister[1], Angela S. Qian[1,3], Jose L. Uribe[1], Rachel W. Martin[1,2]

University of California, Irvine, Department of Chemistry, Irvine, CA 92617University of California, Irvine, Department of Molecular Biology and Biochemistry, Irvine, CA 92617University of California, Irvine, Department of Physics and Astronomy, Irvine, CA 92617

Solid state nuclear magnetic resonance (ssNMR) spectroscopy is invaluable for studying organic compounds, inorganic solids with quadrupolar nuclei, and biological samples such as membrane-bound proteins.[1] The ssNMR *probe* is essential instrumentation for studying these compounds, sending radiofrequency (RF) pulses to and transmitting signals from samples in the RF coil.[1] Development of ssNMR probes has historically used specialized electronic components and expensive CNC machines requiring a niche skillset.[1,2] In contrast, additive manufacturing (3D-printing) is a more affordable and accessible fabrication method.[3] By fabricating an almost completely 3D-printed NMR probe, we will provide a new low-cost route to produce ssNMR probes. These methods can enable other labs to produce custom probes for chemical analysis that may have been previously limited by cost or machining. A ^{1}H-^{31}P 500 MHz ssNMR probe will be made based on a tuning-tube model with short pieces of coaxial transmission-line as the tune and match elements. This work looks at the probe in a two-prong approach: *conductive* components and *dielectric* components. *Conductive* components were modularly designed to fit 3D-printing constraints and produced using copper lost wax casting (Shapeways; Eindhoven, NLD) or fused deposition modeling (FDM) 3D-printing followed by low-cost catalytic metallization and electroplating.[4] The conductivity of metallized 3D-printed parts will be compared to commercial OFHC copper. Next, the *dielectric* components for the probe tune and match elements were designed. A 3D-printed tool was developed to test dielectric properties of common 3D-printed materials. Successful development of these components provides a simpler, cost-efficient route toward building custom 3D-printed ssNMR probes.
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Jeffrey Dykstra - University of California, Irvine
1102 Natural Sciences 2, University of California Irvine, CA, 92617 United States, Email: dykstraj@uci.edu

Molecular-level Insights into Biomineral Interfaces Revealed by Solid-state NMR

Mounesha N. Garaga,[1] Sophie F. Young,[1] Alexander P. Plonski,[1] Galia T. Debelouchina[1]

Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA, 92037

The accumulation of biominerals such as hydroxyapatite (HAP) and whitlockite (WHT) is associated with pathological calcification in several neurodegenerative diseases. Studying their surface interactions with small molecules such as amino acids provides valuable insights into the calcification process. In this work, we used multinuclear solid-state NMR detecting ^{13}C, ^{31}P, ^{43}Ca and ^{25}Mg nuclei to characterize the local environments of the amino acids, phosphate frameworks, calcium and magnesium sites, respectively. Two dimensional (2D) ^{1}H-detected experiments under fast MAS were used to probe molecular-level interactions between small molecules and biominerals. In addition, dynamic nuclear polarization (DNP) MAS NMR was employed to enhance the sensitivity, overcoming the limitations of standard solid-state NMR associated with low concentration of small molecules. This enabled access to site-specific information particularly in the carbonyl region, for example in $^{13}C^{1}H$ FSLG-HETCOR experiments. This work demonstrates an NMR-based approach to probe interfacial mechanism of small molecules binding to the surface of biominerals involved in pathological calcification.

Mounesha Garaga Nagendrachar - University of California San Diego
9325 S Scholars Drive, Tata hall, B400 La Jolla, CA, 92093 United States, Email: mgaraganagendrachar@ucsd.edu

Benchmarking DFT and Machine Learning for ^{19}F NMR Crystallography

Mohit Gupta[1], Leonard J. Mueller[1], Joshua D. Hartman[1]

1. University of California Riverside, Department of Chemistry, Riverside, CA 92521, USA

As a spin-1/2 nucleus with 100% natural abundance, high magnetogyric ratio, and a large chemical shift range, ^{19}F is an ideal probe for both biomolecular and materials NMR and NMR crystallography. While it is an ideal target for NMR crystallography, accurate structural assignment requires precise DFT-based shift predictions. We present a computational benchmark of 29 crystalline organofluorines, combining plane-wave GIPAW geometry optimizations with fragment-based hybrid DFT chemical shift calculation. We also evaluate the UMA-M machine-learned potential as a high-speed surrogate for DFT geometry optimization. By establishing a rigorous relationship between computed shielding tensors and experimental shifts, this framework provides a reliable foundation for the structural characterization of both unknown fluorinated materials and complex protein systems.

Mohit Gupta - University of California Riverside
23666 Hemlock Ave APT 40 Moreno Valley, California, 92557 United States, Email: mgupt026@ucr.edu

Microwave Resonator for Nitrogen Vacancy Spin Control in High-Field NMR

Himanshi Himanshi[1,2], Bryan Richards[1,2], Janis Smits[2], Andrew McDowell[3], Sean Lourette[4], Andrey Jarmola[4], Victor Acosta[1,2]

1. University of New Mexico, Department of Physics and Astronomy, Albuquerque, NM USA
2. University of New Mexico, Center of High Technology Materials (CHTM), Albuquerque, NM USA
3. NuevoMR, LLC, 3408 Constitution Ave. NE, Albuquerque, NM
4. Department of Physics, University of California, Berkeley, CA
ODMR Technologies Inc., El Cerrito, CA

Microfluidic nitrogen vacancy (NV) center based NMR spectroscopy can achieve higher spectral resolution with magnetic fields B_0 >1 Tesla. This necessitates driving NV magnetic sublevel transitions with microwave frequencies in the Ka-band. Therefore, we're designing an improved planar microwave resonator capable of coherent NV spin control at 32 GHz with a Rabi frequency of >10MHz.

Himanshi Himanshi - University Of New Mexico
210 Yale Blvd NE Albuquerque, NEW MEXICO, 87106 United States, Email: himanshi@unm.edu

Advanced DFT Models of ^{13}C Chemical Shift Tensors of Organic Crystals

Robbie Iuliucci, Anand Karamcheti, and Ramaniah Karamcheti

Chemistry Department, Washington &; Jefferson College, Washington, PA 15301

Interpreting chemical shifts in terms of structural parameters requires accurate quantum mechanical models that account for both the local electronic environment and the extended crystalline lattice. In this work, we explore multiple levels of density functional theory, including GGA, meta-GGA, hybrid, and double-hybrid functionals, with emphasis on the Perdew–Burke–Ernzerhof family, applied to the Grant single-crystal NMR dataset. This dataset, composed of experimental ^{13}C chemical shift tensors from polyaromatic hydrocarbon and saccharide crystals, provides a rigorous testing ground for evaluating theoretical models of organic solids.
To efficiently exploit higher levels of DFT, we use a monomer-correction strategy that separates lattice and molecular electronic-structure contributions. The extended crystal environment is captured using periodic plane-wave DFT, while orbital-based hybrid and double-hybrid calculations are performed on molecular fragments. The resulting corrected tensors are compared with experimental principal components, isotropic shifts, and tensor anisotropies to assess the accuracy of each theoretical model.
By combining periodic lattice calculations with higher-level molecular electronic-structure methods, this approach provides a practical route for improving the prediction of ^{13}C chemical shift tensors in organic crystals. The results will help define the level of theory required to reproduce experimental chemical shifts with near-ppm accuracy and will guide future applications of NMR crystallography to molecular solids of increasing complexity.

Robbie Iuliucci - Washington & Jefferson College
60 S. Lincoln St. Washington, PA, 15301 United States, Email: riuliucci@washjeff.edu

Optical Detection of Nuclear Spin Ensembles in Diamond with NV centers

Andrey Jarmola,1, 2 Maxwell D. Aiello,3, 4 Janis Smits,3 Yaser Silani,3 Andris Berzins,3 David Lidsky,3 Bryan A. Richards,3, 4 Amilcar Jeronimo Perez,3, 4 Chandrasekhar Ramanathan,5 Sebastián C. Carrasco,6 Jabir Chathanathil,6 Michael Goerz,6 Vladimir Mal

1. Department of Physics, University of California, Berkeley, CA 94720, USA
2. ODMR Technologies Inc., El Cerrito, CA 94530, USA
3. Center for High Technology Materials, University of New Mexico, Albuquerque, NM 87106, USA
4. Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM 87106, USA
5. Department of Physics and Astronomy, Dartmouth College, Hanover, NH 03755, USA
6. DEVCOM Army Research Laboratory, Adelphi, MD 20783, USA
7. Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany
8. Helmholtz-Institut Mainz, 55099 Mainz, Germany

Nuclear spin ensembles in diamond are promising candidates for quantum sensing applications, including rotation sensing. Direct optical initialization and readout of the intrinsic ^{14}N nuclear spins associated with nitrogen-vacancy (NV) centers in diamond have been used to demonstrate the operation of a rotation sensor[1]. However, the performance of such a system is limited by the relatively low spin density, as there is only one intrinsic ^{14}N spin for each NV electron spin. Here, we introduced a method for optical detection of large ensembles of coherent ^{13}C nuclear spins in diamond[2]. This method is based on microwave-swept dynamics that bidirectionally transfer polarization between NV electron and ^{13}C nuclear spins. We used it to demonstrate optically detected nuclear magnetic resonance (ODNMR) spectroscopy at low magnetic fields (? 10 mT) and ambient temperature. Compared to prior diamond ODNMR experiments using the intrinsic ^{14}N nuclear spin associated with NV centers, the present method allows for the measurement of a larger number of nuclear spins and operation in a broad range of magnetic fields. With further optimization, this approach may find application in fundamental physics tests or in compact rotation sensors.
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Andrey Jarmola - UC Berkeley
366 LeConte Hall #7300 Berkeley, CA, 94720-7300 United States, Email: jarmola@berkeley.edu

Structure of Isolated Yttrium Sites in Dealuminated Beta Zeolites

Dulani K. Kumarasinghe,[1] Jayasubba Reddy Yarava,[1] Young Gul Hur,[2] James W. Harris,[2] Amrit Venkatesh.[1]

1. Department of Chemistry, University of Virginia, Charlottesville, VA 22904
2. Department of Chemical and Biological Engineering, University of Alabama, Tuscaloosa, AL 35487

Yttrium-modified dealuminated beta-zeolite (Y-deAlBeta) materials have garnered attention as catalysts for upgrading biomass-derived oxygenates by enhancing Lewis acidity, for example in ethanol to butadiene conversions.[1-3] Recently, Lin et al. showed that Yttrium incorporation primarily occurs at Q3 silanol sites ((HO-Si-$(OSi)_3$) using ^{29}Si single pulse magic angle spinning (MAS) NMR experiments.[2] However, the local structure of Yttrium sites in Y-deAlBeta is still poorly understood, limiting approaches to enhance catalysis. Here, we directly probe the local environment of Yttrium active sites using multinuclear ^{89}Y, ^{29}Si, and ^{1}H solid-state NMR. Although ^{89}Y is a 100% abundant, spin-1/2 nucleus, ^{89}Y resonates at a very low Larmor frequency of 2.09 MHz/T, resulting in poor NMR sensitivity. This problem is exacerbated in heterogeneous materials such as Y-modified deAlbeta, where a distribution of coordination environments broadens ^{89}Y NMR linewidths. Here, we mitigate these challenges in two ways. First, cross polarization with Carr-Purcell-Meiboom-Gill (CP-CPMG) detection enabled the observation of ^{89}Y solid-state NMR spectra of 3 and 10 wt.% Yttrium loaded Y-deAlbeta at 18.8 T and 10 kHz MAS frequency. Furthermore, proton detection at fast MAS frequencies of 50 kHz enabled ^{1}H-^{89}Y correlation spectra at 14.1 T that showed ^{1}H sites proximate to Y sites in the structure. In addition, fast MAS two-dimensional (2D) ^{1}H-^{1}H and ^{1}H-detected ^{1}H^{29}Si Lee-Goldburg CP spectra allowed us to establish the speciation of protons near Y. These approaches enable a detailed understanding of local structure of isolated Y sites in Y-deAlBeta, highlighting the potential of solid-state NMR to probe isolated single atom sites in heterogeneous catalysts.

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Dulani Kumarasinghe - University of Virginia
Department of Chemistry, University of Virginia, Charlottesville, Virginia, 22904 United States, Email: wde2je@virginia.edu

NMR-Assisted Crystallography of Aspartate Aminotransferase: Protonation States and Catalytic Mechanism

Paula M. Magat[1], Jacob B. Holmes[1], Christopher G. Williams[1], Rittik K. Ghosh[1], Leonard J. Mueller[1]

[1] University of California, Riverside, Department of Chemistry, Riverside, CA 92521

Pyridoxal-5'-phosphate (PLP)-dependent enzymes comprise approximately 4% of all classified enzymes and catalyze a remarkable range of reactions, including transamination, racemization, decarboxylation, and carbon rearrangements.[1] Despite their prevalence and importance, the molecular origins of reaction specificity among PLP-dependent enzymes remain incompletely understood.[2] Increasing evidence suggests that protonation states within the active site play a central role in controlling catalytic function.[3] Aspartate aminotransferase (AAT), a model PLP-dependent enzyme, utilizes finely tuned protonation equilibria to stabilize carbanionic intermediates during the reversible transamination of dicarboxylic amino acids and ketoacids.[4] However, direct determination of hydrogen atom positions and protonation states remains challenging using conventional structural biology techniques.

To address this limitation, we employ NMR-assisted crystallography, integrating solid-state NMR spectroscopy, diffraction-based structural methods, and quantum chemical calculations to investigate the active-site chemistry of AAT at atomic resolution. High-resolution ^{13}C and ^{15}N solid-state NMR spectrum were acquired using a Bruker CryoMAS probe, whose exceptional sensitivity enabled the detection and assignment of key isotopically labeled sites within the PLP cofactor, substrate analogs, and active-site residues. The enhanced signal-to-noise afforded by the CryoMAS provided critical chemical-shift information from ionizable groups, particularly the Schiff base and pyridine nitrogens, allowing protonation states and substrate-induced perturbations to be monitored in detail.

Experimental chemical shifts were combined with first-principles quantum chemical calculations and cluster models derived from crystallographic structures to evaluate candidate protonation-state models. This integrated approach refines structural descriptions of short-lived catalytic intermediates, improves hydrogen localization, and reveals how active-site protonation governs PLP reactivity and reaction specificity. Together, these results provide a chemically detailed framework for understanding PLP-mediated transamination and establish a foundation for future enzyme engineering, mechanistic studies, and rational inhibitor design.

Paula Magat - University of California, Riverside
501 W Big Springs Rd. Riverside, CALIFORNIA, 92521 United States, Email: pmaga003@ucr.edu

NMR-Assisted Crystallography of Aspartate Aminotransferase: Protonation States and Catalytic Mechanism

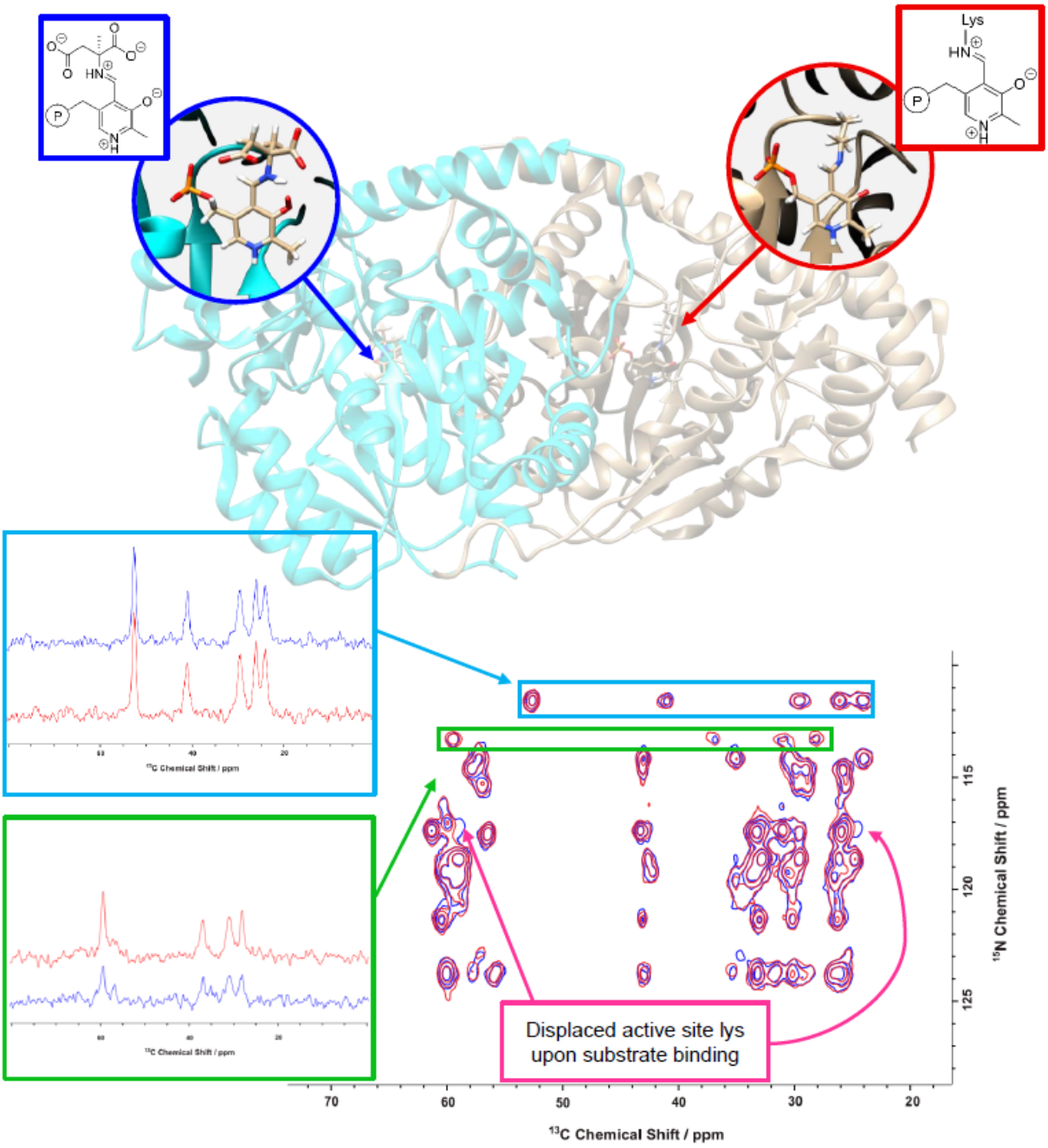

Figure 1: Joint x-ray/neutron structure of AAT asymmetric homodimer (PDB 5VJZ).[5] 2D NC spectra of [^{13}C, ^{15}N]-Lys labelled AAT showing correlations from amide backbone to side chain carbons. Loss of intensity in the active site lysine (green box), with respect to the other lysine residues (blue box) indicates reaction with substrate analogue, 2-methylaspartate.

Tracking Electrolyte Decomposition and SEI Formation in Lithium ion Batteries Using *Operando* ^{19}F NMR

Emma G. Magee,[1] Kevin J. Sanders,[1] Gillian R. Goward[1]

Department of Chemistry, McMaster University, Hamilton, Ontario, Canada

Lithium-ion batteries remain at the forefront of rechargeable energy-storage technologies due to their high energy density. To achieve optimal performance, cells need to be charged to voltages beyond the stability of conventional carbonate-based electrolytes.[1] As a result, electrolyte reduction occurs at the anode during charging, leading to the formation of a passivating layer known as the solid electrolyte interphase (SEI). The SEI is an evolving matrix composed of a wide range of lithium- and non-lithium-containing compounds.[2]

SEI pulverization caused by anode volumetric changes, as well as lithium plating caused by high lithium-ion concentrations at the anode surface, leads to continuous SEI reformation and further active-lithium consumption.[3] Lithium lost by SEI growth is indistinguishable from lithium plated on the anode when evaluated solely through capacity measurements. While nuclear magnetic resonance (NMR) is widely used to distinguish SEI components and electrolyte reduction by-products, the mechanisms governing SEI formation and evolution during cycling remain poorly understood.

Electrolyte reduction species alter the local chemical environment of the hexafluorophosphate anion, to which ^{1}?F T1 relaxation is highly sensitive. Using *operando* NMR, T1 values measured every 30 minutes during C/20 cycling, enable time-resolved tracking of electrolyte decomposition and SEI evolution. An initial T1 increase during the first lithiation reflects electrolyte degradation, while a gradual decrease and oscillation suggest SEI growth and “breathing.” A sharp T1 decrease near 0.23 V during delithiation highlights strong electrochemical dependence of the fluorine environment. Collectively, these results demonstrate that *operando* ^{1}?F T1 relaxation provides a sensitive, non-invasive, real-time technique to probe both electrolyte decomposition and local environmental changes, offering new insight into SEI formation and evolution.

Emma Magee - McMaster University
1280 Main Street West Hamilton, ON, L8S 4L8 Canada, Email: mageee@mcmaster.ca

Fast and accurate NMR crystallography with Machine Learning Interatomic Potentials

Shubha S. Gunaga,[1] Robert W. Schurko, [1,2] Sean T Holmes,[1,2] Frederic Mentink-Vigier[1,2]

[1]National High Magnetic Field Laboratory, Florida State University, 1800 E. Paul Dirac Dr, Tallahassee, FL, 32310, USA.
[2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306, USA.

Nuclear magnetic resonance (NMR) crystallography is a robust method for structure determination, but its reliance on costly density functional theory (DFT) for geometry refinement limits its speed and accessibility. While machine learning tools such as ShiftML3 predict magnetic shieldings in seconds,[1] they still require high-quality input geometries, typically obtained from slow DFT optimizations. Herein, we demonstrate that machine learning interatomic potentials (MLIPs) eliminate this bottleneck for organic crystals. Interestingly, models trained on gas-phase molecules at the hybrid ?B97M-V level (OMol25 dataset)[2] — such as UMA-*omol*[3] and MACE-Polar-1[4] — deliver structural quality rivaling hybrid periodic-DFT, without requiring large computational resources. The resulting MLIP–ShiftML3 workflow reduces computational cost by at least three orders of magnitude relative to DFT-based methods, making high-accuracy NMR crystallography accessible without HPC infrastructure, and opening the door to rapid molecular dynamics simulations at the hybrid DFT level. Combined with sensitivity enhancement via dynamic nuclear polarization (DNP), we demonstrate the approach on L-histidine, extracting the ^{13}C and ^{1}5N chemical shift tensors, and ^{1}H chemical shifts, at natural isotopic abundance and discriminating between its monoclinic and orthorhombic polymorphs.
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Frederic Mentink-Vigier - National High Magnetic Field Laboratory
1800 E Paul Dirac Dr Tallahassee, Florida, 32310-3706 United States, Email: fmentink@fsu.edu

Structural Analysis of ^{13}C and ^{15}N Isotopically Labeled Chitin in its Natural Biological State via Solid-State NMR of *Manduca sexta* Pupal Cuticle

William A. Nese,[a] Juliana R. Burnside,[a] Sean Holmes,[b] Shubha S. Gunaga,[b] Frederic Mentink-Vigier,[b] and Terry Gullion[a]

a. West Virginia University, C. Eugene Bennett Department of Chemistry, Morgantown, WV 26506-6045
b. National High Magnetic Field Laboratory and Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32310

Chitin is ubiquitous among insects and other arthropods and is the second most abundant biopolymer. This polysaccharide, in many ways, is responsible for the success of insects since it is a major component of insect wings and exoskeletons.[1,2] The structure of chemically isolated chitin was determined via X-ray crystallography by Minke and Blackwell and later refined by Sikorski, Hori, and Wada.[2,3] Our recent solid-state NMR and DFT work found new structural conformations in isolated chitin that were not detected by previous studies, and these results will be discussed. In its natural biological state, chitin is part of a protein/chitin matrix.[1,4,5] Therefore, the question that naturally arises is what the structure of chitin in its native state is and how it differs from that when chemically isolated. To address this question, we have embarked on a study of chitin in the pupal cuticle of the tobacco hornworm (*Manduca sexta*). This study entails ^{13}C and ^{15}N isotopic enrichment of chitin to facilitate NMR methods such as REDOR, TEDOR, and homonuclear correlation experiments. A description of labeling procedures will be provided and preliminary NMR results of labeled chitin in its native state will be presented. The long-term objective is to gain a better understanding of the unique mechanical and chemical properties of chitinous components of insects.

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William Nese - West Virginia University
100 Prospect Street, Morgantown, WV 26506 United States, Email: wan00004@mix.wvu.edu

Solid-State NMR and DNP Investigation of PFAS Binding in Zr-Based MOFs

Kunyu Wang,1 Duhan Zhang,2 Yaojun Zeng,1 Ashley Beers,2 Jochem Struppe,3 Daniel Banks,3 James Kempf,3 Yifan Quan,2, * and Shu Yang1

1Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA 19104, USA
2Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA
3Bruker Biospin, Billerica, MA 01821, United States

Metal-organic frameworks (MOFs) are crystalline materials with nanosized pores for transporting energy and matters, based on the interconnection of metal nodes and organic liagnds. Engineering their pore environments at nanoscale can facilitate the ingress of guest molecules and broaden their practical applications. Herein, we have developed a Zr-based MOF consisting of accessible binding sites to accommodate per- or poly-fluoroalkyl substance (PFAS), which are emerging contaminants widely
observed in drinking water in the US. Benefiting from the hierarchical porosity of the MOF, it is able to remove > 90% perfluorooctanoic acid (PFOA) in water within 1 min, which paves the pathway for real-world applications in water purification. Furthermore, the strong coordination bond between Zr atoms and carboxylate groups ensures the high chemical stability of the MOF, which can remain robust
in strong acid for 24 hours.
To directly probe host-guest interactions, we performed solid-state NMR experiments at 500 MHz using a 1.3 mm HFX MAS probe. 1H MAS and 13C CP-MAS spectra of PFOA-loaded MOF suggest deprotonation upon adsorption and formation of coordinated carboxylate species, with additional stabilization via hydrogen bonding. Two-dimensional 19F-1H HETCOR experiments provide direct spatial correlations between MOF hydroxyl protons and both CF2 and CF3 groups. These data support a model in which PFOA is confined within the MOF pores, anchored via its headgroup to Zr6 clusters, while the fluorinated chain extends into the pore and interacts with the framework. This host-guest structure is further supported by density functional theory (DFT) calculations.
19F DNP is a powerful approach to studying PFAS adsorption. DNP experiments were performed at 400 MHz using AMUPOL as the polarizing agent. A 1H enhancement of e ˜ 32 was achieved, whereas the 19F enhancement remains limited (e ˜ 3), underscoring the need for HFX probe to improve sensitivity in 19F-detected experiments.

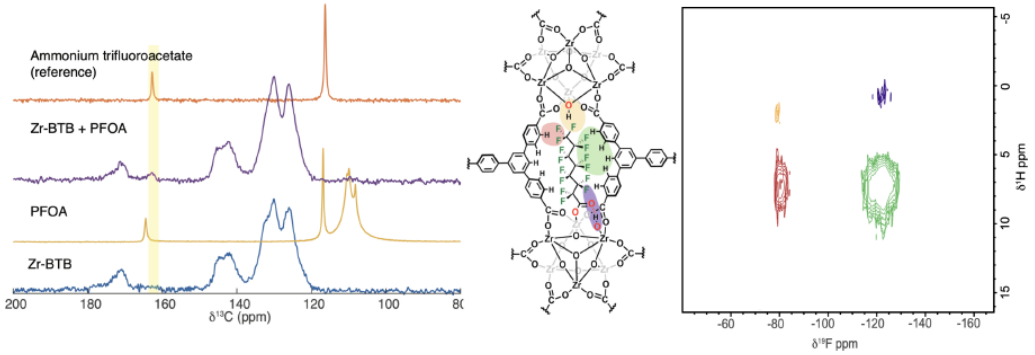

FIG. 1: Solid-state NMR characterization and proposed binding mode of PFOA within the Zr-based MOF. (**Left**) ^{13}C CP-MAS spectra. The shift of the PFOA carboxyl carbon upon adsorption indicates deprotonation and coordination to Zr_6 clusters. (**Center**) Schematic illustration of the host–guest binding configuration, showing coordination of the PFOA carboxylate headgroup to open Zr sites and confinement of the fluorinated chain within the pore. (**Right**) ^{19}F-^{1}H HETCOR spectrum, revealing spatial correlations between MOF hydroxyl protons and CF_2/CF_3 groups.

Yifan Quan - University of Pennsylvania
231 S. 34 Street Philadelphia, PA, 19104 United States, Email: yquan@sas.upenn.edu

Triple-Resonance (HFX) Enables Separation of ^{19}F-Mediated Cross-Relaxation Pathways under DNP

Edvards R. Bensons,[1] César Själsjö,[2] Björn Corzilius[1,3]

1. Univeristy of Rostock, Institute of Chemistry and Department Life, Light &; Matter, Rostock, 18059 Germany
2. Swedish NMR Centre, University of Gothenburg, Gothenburg, 413 90 Sweden
3. Leibniz Institute for Catalysis, Rostock, 18059 Germany

In solid-state NMR, dynamic nuclear polarization (DNP) is a versatile hyperpolarization method, with a wide range of applications ranging from structural biology to materials science. To fully leverage the potential of DNP, it is required to investigate and understand the polarization pathways involved in hyperpolarizing the sample. One such pathway is based on ^{1}H-^{13}C cross-relaxation (CR) induced by methyl groups. This is utilized in SCREAM-DNP (specific cross-relaxation by active motions und DNP) and allows to observe ^{13}C resonances in spatial proximity to the dynamic functional group.[1]
In this work we expand the SCREAM-DNP methodology to CF_3 groups in different chemical environments to explore ^{19}F-mediated heteronuclear CR pathways. In this regard, we have developed a four-block experiment that can disentangle the different pathways by selective saturation of either ^{1}H, ^{19}F, or both spin species simultaneously. Due to the technical requirements of irradiating both ^{1}H and ^{19}F this approach is only accessible with a dedicated H/F/X LTMAS DNP probe.[2]With this, we have been able to isolate the different contributions on three different fluorinated small molecules and in all cases observed a ^{19}F-^{13}C CR pathway. Furthermore, in intramolecular presence of protons we additionally observed a ^{1}H-^{13}C as well as a ^{1}H-^{19}F-^{13}C pathway showing that mere proximity to the CF_3 group is sufficient to induce CR between ^{1}H and ^{13}C even without using ^{19}F as an intermediate recipient of hyperpolarization. The three-spin-pathway (^{1}H-^{19}F-^{13}C) is of high interest due to its high site-specificity, and we anticipate it to be valuable for the further development of dedicated DNP experiments.

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Edvards Roberts Bensons - University of Rostock
Albert-Einstein-Straße 27 Rostock, Mecklenburg-Western Pomerania, 18059 Germany, Email: edvards.bensons@uni-rostock.de

Determination of Atomically Precise Models of CdSe Quantum Dots Using DNP-Enhanced REDOR Solid-state NMR Spectroscopy.

Anuluxan Santhiran,[1, 2] Jie Zhu,[4] Xueqian Kong,[5] Xiaogang Peng,[4] Javier Vela,*[1, 2] Frédéric A. Perras,*[1, 2, 3] and Aaron J. Rossini*[1, 2]

[1]Division of Materials Science and Engineering, Ames National Laboratory, Ames, Iowa, USA 50011.
[2]Department of Chemistry, Iowa State University, Ames, Iowa, USA 50011.
[3]Division of Chemical and Biological Sciences, Ames National Laboratory, Ames, Iowa, 50011, United States.
[4]Key Laboratory of Excited-State Materials of Zhejiang Province and Department of Chemistry, Zhejiang University, Hangzhou, 310027, China.
[5]Institute of Translational Medicine, Shanghai Jiao Tong University, Shanghai, 200240, China.

Quantum dots (QDs) have been widely investigated due to their unique optoelectronic properties. Their photophysical properties can be modulated and optimized by surface ligand or by growing an inorganic shell. Therefore, there is a critical need to understand the atomic-level structure of QD surfaces and interfaces. Here, we show that multinuclear rotational-echo double-resonance (REDOR) solid-state NMR experiments can be used to measure heteronuclear distances in CdSe QDs. We have performed DNP-enhanced $^{13}C^{77}Se$, $^{77}Se^{13}C$, and $^{13}C^{111}Cd$ REDOR experiments to probe the heteronuclear distances between carbon, selenium, and cadmium. The INTERFACES[1] computer program can be used to quickly and accurately simulate the REDOR dephasing curves. Based upon this analysis, we conclusively show that the QDs have a zinc blende crystal structure with a dense network of chelating carboxylate ligands coordinated to surface Cd atoms. These experiments can also be applied to determine precise structural models of CdSe/CdS core/shell QDs, where REDOR enables the ratio of sulfur and selenium atoms within the first few layers of each QD to be determined.
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Anuluxan Santhiran - Iowa State University
Pammel Drive Ames, IA, 50011 United States, Email: anuluxan@iastate.edu

Probing the Size Dependence of Knight Shifts in Doped Cadmium Oxide Nanocrystals Using ^{113}Cd and ^{139}La Solid-State NMR

Robert B. Smith[1,2], Sophie A. Boglaev[1,2], Ali Pazoki[1], Adham Maher[1], Geoffrey F. Strouse[1], Robert W. Schurko[1,2*†]

1. Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL, 32306
2. National High Magnetic Field Laboratory, Tallahassee, FL, 32310
† Presented posthumously (deceased February 2026)

Transparent conducting oxides (TCOs) are of great interest because of their high infrared reflectance, visible transparency, and tunable electrical conductivity.[1] Cadmium oxide (CdO) nanocrystals (NCs), one of the most commonly used TCO NCs, is an intrinsic *n*-type semiconductor (*i.e.*, electrical conductivity is present without the introduction of a dopant) with a wide band gap of *ca*. 2.2 eV, low resistivity, and high optical transparency typical of TCOs.[2] Manipulating the size of CdO NCs allows for tuning of these properties, yielding performance comparable to that of established TCOs. An understanding of the relationships between atomic-level structure and these tunable properties is crucial to the rational design of novel TCOs and modification of existing TCOs. Solid-state NMR (SSNMR) spectroscopy is a valuable tool in this respect, as its sensitivity to local atomic environments allows for selective probing of different regions of the NC, allowing for detailed comparisons to be drawn between local structure, the nature of the band gap, and the generation of free carriers.[3-5] SSNMR of metal nuclides in TCOs is of particular value, since measurement of chemical shift anisotropies and Knight shifts can lend insight into the aforementioned structural features. Crucially, Knight shifts provide direct evidence of how differences in NC structure impact free carrier densities and band gaps.[6] Herein, I describe the use of ^{113}Cd (I = 1/2) SSNMR to study a series of tin-doped CdO NCs varying in size, with the goal of differentiating the NC surface from the core through use of Knight shifts. T_1(^{113}Cd) relaxation rates are used to gain insight into the distribution of free carriers throughout the NC and the presence of Korringa-like behavior.[7,8] I will also present preliminary data using ^{113}Cd and ^{139}La (I = 7/2) SSNMR to study a series of lanthanum-doped CdO NCs.

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Robert Smith - Florida State University/National High Magnetic Field Lab
102 Varsity Way Tallahassee, Florida, 32304 United States, Email: rs20hl@fsu.edu

Pushing the Limits: Resonance Assignment of a 144 kDa Enzyme via 1.1 GHz NMR

Alexander F. Thome,[1] Christopher G. Williams,[1] Songlin Wang,[2] Owen A. Warmuth,[3] Chad. M. Rienstra,[2,3] Leonard J. Mueller[1]

Department of Chemistry, University of California-RiversideNational Magnetic Resonance Facility at Madison (NMRFAM), University of Wisconsin-MadisonDepartment of Biochemistry, University of Wisconsin-Madison

We report on the resonance assignment of the 144 kDa microcrystalline U- ^{13}C,^{15}N- labeled tryptophan synthase ("TS", 2x72 kDa) at 1.1 GHz. At ultrahigh field, we have identified over 590 unique amino acid spin-systems, with 242 of the 665 total residues having been assigned to the a and ß-subunit backbones thusfar. These assignments are enabled in part by Long-Observation-Window Band-Selective Homonuclear Decoupling (LOW-BASHD), which removes scalar coupling to C^a during carbonyl detection to enhance resolution in the direct dimension. To complement to these experiments, we report additional MAS Cryoprobe (600 MHz) correlation spectra of microcrystalline TS with a unique U-^{13}C,^{15}N-histidine, U-^{13}C,^{15}N-lysine double-labeling scheme. These emerging experiments facilitate direct observation of site-specific histidine protonation states while also assisting the goal of near-complete assignments.

Alexander Thome - University of California-Riverside
950 W Linden Street, Apartment 28 Riverside, CA, 92507 United States, Email: athom162@ucr.edu

Towards Microscale NMR at 14T using Quantum Diamond Sensors

Chun Tung Cheung1, Emmeline Riendeau1, Zhiran Zhang
2, Evan Villafranca2, Ian Hammock2, Nazar Delegan2,3, F
Joseph Heremans2,3, Alexander A High 2, Joseph R
Sachleben 4 , Peter Maurer 2

1. Department of Physics, University of Chicago
2. Pritzker School of Molecular Engineering, University of Chicago
3. Material Science Division, Argonne National Laboratory
4. Biomolecular Nuclear Magnetic Resonance Facility, University of Chicago

Quantum sensors are driving the miniaturization of NMR spectroscopy toward the single-molecule level. Recent advances in quantum sensing based on Nitrogen-vacancy (NV) centers have demonstrated nm-scale NMR, mHz spectral resolution, and sub-pT/Hz sensitivity, raising hopes for NMR analysis of single biomolecules. However, early NV-NMR experiments focused on proof-of-principle demonstrations at low magnetic fields ($<3T$), which limited spectral resolution; a strong field is essential to resolve chemical shifts for molecular structure analysis.

Here, we tackle the formidable task of engineering an NV-NMR spectrometer at $14T$, converging disciplines from THz engineering, diamond material science, high-field quantum sensing, and lab-on-a-chip integration. We developed quantum control at $14T$, driving $8MHz$ Rabi oscillations of NV centers at $398GHz$ using planar metal THz metamaterials. We achieved NV-doping on (111)-cut diamond substrates using MPCVD, creating a thick layer of dense NV ensembles. Furthermore, we demonstrated sensing protocols at $14T$, showing AC magnetometry with $100nT/Hzm^3$ sensitivity. We integrated a microfluidic system with the diamond sensor chips, allowing the delivery and control of $20pL$ of analyte to the assay site.

Our $14T$ NV-NMR spectroscopy system is enabling us to resolve spectra from microscale samples with chemical specificity. This eventually allows NV-NMR to move beyond the laboratory toward real-world biochemical applications, paving the way for single-cell metabolomics, drug engineering, and beyond.

Chun Tung Cheung - University of Chicago
5640 S Ellis Ave, WERC LL250F Chicago, IL, 60637 United States, Email: ctcheung1123@gmail.com

Solid-State NMR to Elucidate Interactions of Small Molecule Fluorescent Dyes with Pathological Calcification Surfaces

Sophie F. Young[1], Alexander P. Plonski[1], Mounesha N. Garaga[1], Leonard Mueller[2], Richard B. Thompson[3], Galia T. Debelouchina[1]

[1]Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA, 92037
[2]Department of Chemistry, University of California, Riverside, Riverside, CA, 92521
[3]Department of Biochemistry and Molecular Biology, University of Maryland School of Medicine, Baltimore, MD, 21201

Aberrant deposition of calcium phosphate minerals in tissues is prevalent in chronic and age-related diseases, including cardiovascular disease, age-related macular degeneration (AMD), and Alzheimer's disease (AD). The precise mechanisms of the calcification process and how key biomolecular players interact with mineral surfaces are poorly understood, however. A variety of small molecule fluorescent dyes are available for the detection of calcification in tissues, but they have poor mineral selectivity and the mechanisms by which they bind to mineral surfaces are unknown. We are applying solid-state NMR to examine how the small molecule dye xylenol orange interacts with calcification minerals at the atomic level. Such mineral-bound samples are difficult to study by conventional NMR due to exceptionally low sensitivity. To overcome these challenges, we are utilizing cryoMAS and dynamic nuclear polarization (DNP). Here, we will report our characterization of xylenol orange and compare its interactions with two pathological calcification minerals, hydroxyapatite and whitlockite. We expect these findings will provide insight into how small molecules interact with distinct mineral surfaces and highlight new avenues for developing improved diagnostic or therapeutic tools that target pathological calcification. Supported by NIH P01 AG081167 and NIH T32 GM146648 (UC San Diego).

Sophie Young - University of California, San Diego
8514 Villa La Jolla Dr. #120 La Jolla, California, 92037 United States, Email: sfy001@ucsd.edu

Interpreting chemical shielding tensors: a well-posed approach through real-space analysis

Josef W. Zwanziger

Department of Chemistry, Dalhousie University, Halifax B3H 4R2, Nova Scotia, Canada

The chemical shielding tensor is the primary object of interest in most NMR studies of solids, both computational and experimental. Using the shielding as a probe of bonding raises several challenges, if more detail is desired than a simple match between calculated values and a set of known test compounds. In particular, there are two types of gauge invariance issues that must be addressed. First, there is the well known gauge of the magnetic vector potential, which can be accommodated in several ways to yield a gauge invariant shielding, although even here ambiguity remains in making artificial separation between contributions, say paramagnetic and diamagnetic terms. Secondly, and probably less widely appreciated, is that the total shielding should be invariant to the choice of orbital decomposition in the interpretation scheme. Such invariance is likely impossible to impose rigorously.

Here we explore an alternative approach, which is well-posed and manifestly gauge invariant (in both senses discussed above), by focusing on the chemical shielding as represented as a density in real space. Our work follows on the pioneering studies of Jameson and Buckingham.[1] We discuss first the source of the gauge issues mentioned above, and demonstrate how and where in interpretations they lead to ambiguities. Then we show how a real-space representation is obtained in a solid-state calculation, and how it may be visualized and analysed, without initial orbital decomposition. Examples will be shown on atoms, molecules, and extended solids.

C. J. Jameson and A. D. Buckingham, J. Chem. Phys., 1980, *73*, 5684.

Josef Zwanziger - Dalhousie University
PO Box 15000 Halifax, NS, B3H 4R2 Canada, Email: jzwanzig@dal.ca

^{1}H led NMR Structure Determination in Molecular Solids

Jacob B. Holmes[1,2], Daria Torodii[1], Ruben Rodriguez-Madrid[1], James J. Kimball[1], Lyndon Emsley[1,2]

[1] Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland
[2] National Centre for Computational Design and Discovery of Novel Materials MARVEL, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.

Rich chemical understanding is critically important to understanding function in all chemical systems. Here, we show how the determination of complete three-dimensional structures can be improved and accelerated for materials at natural isotopic abundance using new experimental methods with >100 kHz MAS, machine-learned chemical shift predictions, and rapid assignment methods, to validate structures within hours. We highlight these advances with the first demonstration of ^{1}H-^{1}H J-couplings in solids, structure validation using only ^{1}H-detected methods, the improvement of ShiftML to DFT accuracy, and the use of probabilistic methods for chemical shift assignment. The methods are combined to determine complete atomic-level structures of disordered molecular solids.

Jacob Holmes - EPFL
Avenue François-Alphonse Forel Lausanne, Vaud, 1015 Switzerland, Email: jacob.holmes@epfl.ch

Structure Determination of 2D Germanane, Methyl Germanane and Methyl Germanane-Stannane Nanosheets by Nuclear Magnetic Resonance Spectroscopy

L.M. Yunusa,[1,2] Jeremy Essner,[3] Maharram Jabrayilov,[3] Abhijit Bera,[3] Bradyn C. Weaver,[1,2] Amrit Venkatesh,[4] Alexander J. Kopeny,[1] Takeshi Kobayashi,[1] Frederic A. Perras,[1,2] Rana Biswas,[1] Ivan Hung,[5] Zhehong Gan,[5] Matthew G. Panthani,[3] and Aaron J. Rossini

[1]Ames National Laboratory, Division of Materials Science and Engineering, Ames, Iowa, USA
[2]Department of Chemistry, Iowa State University, Ames, IA, USA
[3]Department of Chemical and Biochemical Engineering, Iowa State University, Ames, IA, USA
[4]Department of Chemistry, University of Virginia, Charlottesville, VA, USA
[5]National High Magnetic Field Laboratory, Tallahassee, FL, USA

Two-dimensional (2D) germanium-based materials have attracted considerable attention due to their tunable optical and electronic properties and potential applications in atomically thin semiconductor devices.[1] These materials are commonly synthesized by topotactic deintercalation of layered precursors such as $CaGe_2$ or SrGeSn using reagents including hydrochloric acid (HCl) or iodomethane (CH_3I).[2] However, these processes typically results in structurally disordered nanosheets with mixed surface terminations, which limits characterization by single-crystal or powder X-ray diffraction-based methods.[3] Here, we use solid–state nuclear magnetic resonance (NMR) spectroscopy, complemented by energy-dispersive X-ray spectroscopy (EDX), to probe the local structure of hydrogen terminated germanane (H–Ge), methyl terminated germanane (CH_3–Ge), and methyl terminated germanium-tin nanosheets (CH_3–GeSn). EDX analysis indicates that 13%-18% of Ge and Sn atoms are terminated by halogen species (Cl or I), depending on the deintercalation conditions. Interestingly, ~6% of methyl groups in CH_3–Ge are identified as methoxide (CH_3O-Ge), likely formed by hydrolysis of CH_3I. $^{13}CH_3$–GeSn can be easily and inexpensively prepared by using $^{13}CH_3I$ during synthesis. ^{13}C-enrichment of CH_3–GeSn enables $^{13}C^{119}Sn$ REDOR and 2D ^{13}C homonuclear correlation NMR experiments to be performed. These experiments allow carbon-tin and carbon-carbon interatomic distances to be precisely measured. Modeling of $^{13}C^{119}Sn$ REDOR curves using the INTERFACES computer program[4] confirms that CH_3–GeSn consists of a semi-ordered 2D lattice with alternating methyl terminated Ge and Sn atoms. High-field ^{73}Ge NMR further provides insight into the distribution of local electronic environments. The experimental results are in good agreement with plane-wave DFT calculations, providing experimentally validated atomistic models of these disordered materials.

References:

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Lukman Yunusa - Iowa State University
2415 Osborn Dr 1605 Gilman Hall Ames, Iowa, 50011-3111 United States, Email: lmyunusa@iastate.edu

Dynamic Nuclear Polarization with 1.3 mm Diameter Diamond Rotors

Nicholas Wiesner[1], Jiaming Liu[2], Ravi Shankar Palani[1], Samuel Strymish[1], Neil Gershenfeld[2], Robert G. Griffin[1]

[1]Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, United States
[2]Center for Bits and Atoms, Massachusetts Institute of Technology, Cambridge, MA 02139, United States

Magic angle spinning (MAS) nuclear magnetic resonance (NMR) has revolutionized structural biology due to the development of methods to precisely determine bond lengths and torsion angles in medicinally relevant solids such as Aß. Hydrostatic air bearings stabilize small rotors allowing for rotational frequencies over 200 kHz, greatly improving resolution for solid samples. Complementing this technique is dynamic nuclear polarization (DNP) where electron polarization is transferred to local nuclei mediated by microwave excitation. Signal enhancements of ~10^2 are currently routinely achieved. While these techniques can greatly improve resolution and sensitivity, they come with significant operational challenges. The high spinning frequency of MAS rotors may induce structural failure leading to a loss of the sample and causing serious damage to the MAS stator and RF circuitry. Additionally, thick rotor walls absorb microwave power attenuating high DNP enhancements. Currently, most MAS rotors (0.4 mm ? 3.2 mm diameters and larger) are fabricated from zirconia which has high durability but low thermal conductivity and microwave transmissibility. Sapphire rotors, on the other hand, exhibit improved microwave transmissibility and thermal conductivity but low durability. Because sapphire is fragile, rotor diameters are currently limited to = 3.2 mm. In recognition of these drawbacks, our group has recently fabricated 0.7 mm diameter rotors from single crystal HPHT diamond which displays better microwave transmissibility, tensile strength, and thermal conductivity than either of the other two materials.[1] This work includes both the creation of larger, 1.3 mm diamond rotors as well as the first ever DNP experiments to be performed with diamond rotors showing viability as an optimal rotor material.

Schaffer et. al., J. Magn. Res., 2025, *52*, 435.

Nicholas Wiesner - Massachusetts Institute of Technology
77 Massachusetts Avenue Cambridge, Massachusetts, 02139 United States, Email: wiesnern@mit.edu

Probing the limits to refocusing nuclear spin dynamics

Shreyan Ganguly,[1] Chandrasekhar Ramanathan.[1]

1. Dartmouth College, Department of Physics and Astronomy, Hanover NH 03755

Out-of-Time-Ordered Correlators (OTOCs) provide a measure of how a local perturbation propagates through an interacting quantum system. They can potentially be used to study many problems in science, such as characterizing phases of matter and the thermalization of isolated quantum systems. The NMR multiple-quantum coherence (MQC) experiment is a version of an OTOC measurement. It has been suggested that such NMR OTOCS could improve large-scale molecular structure determination[1,2]. A key requirement for exploiting such OTOCs is that the large multi-spin correlations that build up during the NMR experiment have long coherence times and remain controllable. Refocusing the many-body dynamics of a system with high fidelity is key to OTOC measurements. In dipolar-coupled nuclear spin systems this refocusing is done via collective control of the spins. Here we characterize the fidelity of such refocusing and explore the sensitivity of OTOC dynamics to applied perturbation. We experimentally study the growth of MQC correlations in different systems and complement the experimental studies with numerical simulations. High sensitivity to small perturbations serves as a proof of failure of refocusing ability in the system and may establish bounds on the efficacy of OTOC-based studies in these systems. Supported by the Gordon and Betty Moore Foundation, grant DOI 10.37807/GBMF12251 and by Google LLC.
O'Brien et al. PRX Quantum, 3 030345 (2022).Zhang et al. www.arXiv.org:quant-ph/2510.19550.

Chandrasekhar Ramanathan - Dartmouth College
6127 Wilder Laboratory Hanover, NH, 03755 United States, Email: sekhar.ramanathan@dartmouth.edu

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