

RSC ESR 2023 Programme

Monday 27th March		
10:00 - 14:00	Registration	The Edge
13:00 – 14:00	Lunch	The Edge
Commencing of the RSC ESR LEEDS 2023 Conference		
Session Chair: Olav Schiemann		Conference Auditorium
14:00 – 14:10	Christos Pliotas	Welcome
14:10 – 14:50	Enrica Bordignon	Plenary Lecture: Dynamics of the prepore-to-pore transition of a Tc toxin
14:50 – 15:10	Laura Rimmel	Investigating the structure of a fluoride sensing riboswitch by PELDOR and ¹⁹ F ENDOR measurements
15:10 – 15:30	Vasily Oganessian	Understanding the impact of trans-membrane peptides on lipid bilayers by combining EPR with MD simulations
15:30 – 15:50	Dimitri Svistunenko	An EPR account of the Streptomyces lividans dye decolourising peroxidase DtpAa – in the resting ferric haem state and on activation by H ₂ O ₂
16:00 – 17:00	Coffee & Poster Session (Odd numbers)	The Edge – IES
17:00 – 18:00	Coffee & Poster Session (Even numbers)	
IES Prize Session Chair: Songi Han		Conference Auditorium
18:00 – 18:05	Songi Han	Laudatio
18:05 – 18:30	Mantas Šimėnas	IES Young Investigator Award Lecture: EPR with cryogenic amplifiers independent of sample temperature
18:30 – 19:00	IES AGM	IES Committee
19:00 – 20:30	Dinner	The Edge
20:30 – 22:00	JEOL Reception	The Edge
22:00 – Midnight	Hotel Check-In	

Tuesday 28th March		
Session Chair: Maxie Rößler		Conference Auditorium
09:00 - 09:40	Bela Bode	Plenary Lecture: Are nanomolar sensitivity and high-quality computational structures the sunlit uplands of dipolar EPR spectroscopy?
09:40 - 10:00	Sergei Kuzin	Conformational study of barley β -glucan dietary fibers based on the longitudinal spectral diffusion in RIDME
10:00 - 10:20	Annalisa Pierro	SDSL-EPR to tackle the conformational changes of the nascent chain gatekeeper, NAC, at the Ribosome interface
10:20 - 10:50	Coffee	The Edge
Session Chair: Dimitri Svistunenko		Conference Auditorium
10:50 - 11:20	Claudia Tait	Invited Lecture: Increased control of excitation selectivity for pulse EPR on spin-correlated radical pairs with shaped pulses
11:20 - 11:40	Lorenzo Sorace	Exchange-coupled porphyrin complexes as potential molecular quantum gates
11:40 - 12:00	Janko Hergenbahn	Increasing delocalisation by changing the charge state in porphyrin molecular wires
12:00 - 12:20	Alexander Allgaier	Polaron Spin Dynamics in Thin Films of Chemically Doped Semiconducting Polymers
12:20 - 12:30	Bruker Communication	Bruker Team
12:30 - 14:00	Lunch	The Edge
JEOL Prize Session I Chair: Claudia Tait		Conference Auditorium
14:00 - 14:20	Sebastian Kopp	JEOL Student Prize talk: EPR investigation of dynamic and coherent electron transfer in porphyrin radical cations
14:20 - 14:40	Susanna Ciuti	JEOL Student Prize talk: Triplet-radical electron spin polarization transfer in weakly coupled systems
14:40 - 15:00	Ekaterina Shabratova	JEOL Student Prize talk: EPR and X-ray investigations of electronic and structural properties of metal-doped graphitic Carbon Nitride catalysts
15:00 - 15:20	Sebastian Gorgon	JEOL Student Prize talk: Luminescent organic radicals with high-multiplicity excited states
15:20 - 15:40	Short Coffee Break	The Edge
JEOL Prize Session II Chair: Alice Bowen		Conference Auditorium
15:40 - 16:00	Jeannine Grüne	JEOL Student Prize talk: Triplet excitons and associated efficiency-limiting pathways in organic photovoltaics based on non-fullerene acceptors
16:00 - 16:20	Paolo Cleto Bruzzese	JEOL Student Prize talk: Hyperfine spectroscopy for structural characterization of single- metal-atom catalysts with atomic-scale precision. The case of Cu ^{II} -exchanged zeolites
16:20 - 16:40	Hannah Russell	JEOL Student Prize talk: Measuring Nanometre Distance Changes in Biomolecules Under Pressure
16:40 - 17:00	Euan Basse	JEOL Student Prize talk: Characterisation of local environments in strongly paramagnetic battery cathodes: a combined experimental and theoretical approach
17:00 - 18:00	Coffee & Poster Session (Odd numbers)	The Edge - Bridge 12

Session Chair: Janet Lovett		Conference Auditorium
18:00 - 18:30	Maxie Rößler	Invited Lecture: New mechanistic insights into electrocatalytic reactions from film-electrochemical EPR: from <i>ex-situ</i> to <i>in-situ</i> and <i>operando</i>
18:30 - 19:00	RSC ESR AGM	Conference Auditorium
18:30 - 20:00	Dinner	The Edge
Bruker Prize Session		Conference Auditorium
20:00 - 20:10	Claudia Tait	Laudatio
20:10 - 21:00	Stefan Stoll	Bruker Prize Lecture: EasySpin – EPR at your fingertips
21:00 - 22:30	Bruker Reception	The Edge

Wednesday 29th March		
Session Chair: Bela Bode		Conference Auditorium
09:00 - 09:40 APMR Plenary Lecture	Thomas Prisner	Plenary Lecture: PELDOR and ENDOR investigation of structure, dynamics and metal ion binding sites on RNA-motives using rigid spin-labels
09:40 - 10:00	Daniel Klose	Electronic structure of an f-electron-bearing Yb(III) complex from EPR & NMR spectroscopy
10:00 - 10:20	Fabian Hecker	¹⁷ O Hyperfine Spectroscopy Reveals Hydration Structure of Nitroxide Radicals in Aqueous Solutions
10:20 - 10:50	Coffee	The Edge
Session Chair: Emma Richards		Conference Auditorium
10:50 - 11:20	Michal Leskes	Invited Lecture: Paramagnetic metal ions DNP for bulk and surface sensitivity in inorganic solids
11:20 - 11:40	Jan Behrends	Probing Charging and Discharging of Organic Radical Batteries by EPR
11:40 - 12:00	Joseph McPeak	Operando state of charge monitoring of Vanadium redox flow batteries with an EPR-on-a-Chip dipstick sensor
12:00 - 12:20	Yujie Zhao	Testing DNP polarising agents with a high-power EPR spectrometer
12:20 - 13:20	Lunch	The Edge

Session Chair: Christiane Timmel		Conference Auditorium
13:20 - 13:50	Gavin Morley	Invited Lecture: Optically detected magnetic resonance of nitrogen-vacancy centres in diamond for sensitive magnetometry and (eventually) a test of quantum gravity
13:50 - 14:10	Rémi Blinder	Sensitive nuclear magnetic resonance modalities enabled by X-band EPR methods using nanodiamonds
14:10 - 14:30	Joris van Slageren	Molecular qubits: self-assembly and strong coupling
14:30 - 14:50	Michael Franz	Effective Hamiltonian theory to elucidate excited state exchange coupling
14:50- 15:50	Coffee & Poster Session (Even numbers)	The Edge - IoP Magnetism
Session Chair: William Myers		Conference Auditorium
15:50 - 16:20	Thomas Schmidt	Invited Lecture: Quantitative analysis of monomer–dimer equilibrium of the β 1-adrenergic receptor by DEER spectroscopy
16:20 - 16:40	Alessio Bonucci	Investigation on the biogenesis of a multi-protein hetero complex combining cw-EPR and Nitroxide-Gd (III) distance measurements
16:40 - 17:00	Manas Seal	Gd(III)- ^{19}F distance measurements of proteins in cells by electron-nuclear double resonance
17:00 - 17:20	Ciarán Rogers	Spin polarisation in Gd(III) complexes by arbitrary waveform generated excitation pulses for high sensitivity pulsed EPR measurements away from the central transition
17:20 - 17:30	Mini Break	
Bruker Thesis Prize Session		Conference Auditorium
17:30 - 17:40	Gunnar Jeschke	Laudatio
17:40 - 18:20	Nino Wili	Bruker Thesis Prize Lecture: New electron spin resonance experiments with tailored waveform excitation
18:35 - 18:50	ESR Group Photo	Front of Parkinson's Building
18:50 – 19:00	Pick-up (Coaches)	
19:00 - 22:00	Banquet and Drinks	Royal Armouries Museum

Thursday 30th March		
Session Chair: Enrico Salvadori		Conference Auditorium
09:00 - 09:40	Christoph Boehme	Plenary Lecture: Low-magnetic field electrically detected magnetic resonance spectroscopy of electron-hole pairs in thin-film polymer layers
09:40 - 10:00	Christian Dirk Buch	High-field EPR deuteration study of a 4f molecular qubit
10:00 - 10:20	Till Biskup	How reproducible are your EPR results? Tools for fully reproducible data analysis
10:20 - 10:50	Coffee	The Edge
Session Chair: Christopher Wedge		Conference Auditorium
10:50 - 11:20	Akio Kawai	Invited Lecture: Dynamic Electron Polarisation in Radical-Triplet Systems
11:20 - 11:40	Alice Bowen	Light Induced Triplet Triplet Electron Resonance: Optimization, limitations and comparison to other methods
11:40 - 12:00	Naitik Panjwani	Singlet Fission in Lycopene Aggregates Probed by Transient Electron Paramagnetic Resonance Spectroscopy
12:00 - 12:20	Yury Kutin	Characterization of the first ground-state triplet vinylidene
12:20 - 13:10	Lunch and coffee	The Edge
Session Chair: Paul Jonsen		Conference Auditorium
13:10 - 13:30	Enrico Salvadori	Stable and metastable paramagnetic species in carbon nitride
13:30 - 13:50	Yu-Kai Liao	Investigation of the Surface Properties of Microporous Materials Using Nitric Oxide as a Spin Probe
13:50 - 14:10	Muralidharan Shanmugam	Mechanism of Co-C Bond Cleavage in B ₁₂ -Dependent Photoreceptor and the Intermediates probed by Crystallography, UV-Vis and cw-EPR/annealing Methods
14:10 - 14:30	Kavipriya Thangavel	Adsorption of NO on Ni(II)-based MFU-4l catalyst MOF evidenced by EPR spectroscopy and quantum chemical modelling
14:30 - 14:50	Alena Sheveleva	EPR insights into UiO-66 incorporating Cu(II) binding sites for selective adsorption and separation
14:50 - 15:00	Christos Pliotas & Christiane Timmel	Closing Remarks
15:00 - 15:10	Warwick Team	RSC ESR 2024: Warwick
15:10 - 15:20	Poster Removal & End of the RSC ESR LEEDS 2023 Conference	

Satellite Symposium Programme

Monday 27th March		
Heathcote Symposium		Conference Auditorium
11:30 - 11:35	Christos Pliotas	Welcome
11:35 – 11:45	Robert Bittl	Symposium Laudatio
11:45 – 12:15	Peter Heathcote	Symposium Invited talk: Studying photosynthesis and respiration chain proteins by cw and pulsed EPR spectroscopic methods
12:15 – 12:30	Jana Eisermann	The Interplay of ROS production and lipid peroxidation on respiratory complex I
12:30 – 12:45	Yue Ma	Accessing the conformational landscape of the human K2P mechanosensitive channel
12:45 – 13:00	Maria Francesca Vicino	Following conformational changes in LbuCas13a from apo to the ternary cr- and target