

Faraday Joint Interest Group Conference
3-5 April 2023, Sheffield, UK

OVERVIEW PROGRAMME

Friday 31 March 2023 (online only)

14:30	Meet the speakers and RSC prize winners
15:30	PL01 ONLINE PLENARY - Session Chair: Anthony Meijer Coherent chemical dynamics with x-rays Stephen R. Leone, The University of California, Berkeley, USA

Monday 3 April 2023

10:00	Refreshments & registration			
12:00	Lunch & registration			
12:50	Chairs' welcome			
13:00	PL02 PLENARY - Session Chair: Anthony Meijer Engineering metal-organic frameworks functionalities using theory, computation and high-throughput data Laura Gagliardi, University of Chicago, USA			
14:00	Time for delegates to move between theatres			
Theme	Photophysics of functional and solar energy materials	Development of new biophysical methods	New spectroscopic approaches to measuring chemical mechanisms	Measurement of molecules and reactions in complex environments
Session chair	Julia Weinstein	Steven Lee	Caroline Dessent	Andrew Rickard
14:10	PFS03 Computational approaches to design narrow TADF emitter Shawana Ahmad, University of Newcastle, UK	K02 KEYNOTE Revealing protein structure, dynamics and intermolecular interactions in biofluids with 2D-IR spectroscopy Neil T. Hunt, University of York, UK	K03 KEYNOTE Ion-neutral reaction dynamics at low temperatures Brianna Heazlewood, University of Liverpool, UK	K04 KEYNOTE Real-time measurements of reactive intermediates in atmospheric oxidation processes Dan Stone, University of Leeds, UK
14:30	PFS04 A quantitative model for the design of molecules with tuned singlet-triplet energy gaps Felix Plasser, Loughborough University, UK			
14:50	PFS01 Photophysics of bismuth coordination complexes for optoelectronics Bhatia Harsh, University College London, UK	BM01 High-density volumetric super-resolution microscopy Sam Daly, University of Cambridge, UK	NS01 Probing the speciation and electronic structure of organozinc reagents using X-ray spectroscopy Lewis Parker, University of Reading, UK	MM01 Environmental conditions drive self-organization of reaction pathways in a prebiotic reaction network William Robinson, Radboud University Nijmegen, Netherlands
15:10	PFS02 Measuring the extent of dynamical polaron formation and delocalization in photocatalysts Scott Cushing, California Institute of Technology, USA *Online	BM02 Photo-ion mobility mass spectrometry for investigating the structural dynamics of photoreceptor proteins Alex Jones, National Physical Laboratory, UK		MM02 Accurate spectroscopic quantification of the optical properties of nitroaromatic compounds in single aerosol particles Jamie Knight, University of Bristol, UK
15:30	Refreshments			
Theme	Frontiers in excited state chemistry	Astrochemistry and chemistry at cold temperatures	Dynamics of soft matter	Digital chemistry and machine learning
Session chair	Caroline Dessent	Ian Sims	Anthony Meijer	Jiayun Pang
16:00	FES01 Perturbing the photophysics of a sunscreen chromophore Cate Anstötter, University of York, UK	AC01 Probing Enceladus' sub-surface ocean by mass spectrometry: the quest for inorganic and organic biosignatures Bernd Abel, University Leipzig, Germany	SM01 Enhanced accumulation of colloidal particles in microgrooved channels via diffusiophoresis and steady-state electrolyte flows Guido Bolognesi, University College London, UK	DC01 Functional group pair distance-based descriptor for isomerization in porous molecular framework materials Matthew Addicoat, Nottingham Trent University, UK
16:20	FES02 Redefining state-of-the-art in time-dependent density functional theory for core excitations with electron-affinity approaches Kevin Carter-Fenk, University of California, Berkeley, USA	AC02 Metal catalysis in astrophysical environments Victoria Cabedo, ICS-Heriot Watt University, UK	SM02 Focusing and sorting polystyrene particles and liposomes via diffusiophoresis in flat microchannels Adnan Chakra, Loughborough University, UK	DC02 First principles structure and property prediction of energetic materials Joseph Arnold, University of Southampton, UK
16:40	FES03 Joint experimental and theoretical investigation of excited state vibrational coherences in Mn single molecule magnets Julian Eng, Chemistry, SNES - Newcastle University, UK	AC03 On the reaction of simple atoms and ions with ethylene and acetylene on dust surfaces in the ISM Reetu Reetu, University of Sheffield, UK	SM03 Polarisation of water under thermal fields: the effect of the molecular dipole and quadrupole moments Aidan Chapman, Imperial College London, UK	DC03 Machine learning of Gaussian basis sets for use in computational chemistry J. Grant Hill, University of Sheffield, UK
17:00	RSC publishing talk - how to publish with impact When you've done interesting and valuable research you want to share it with the world! This session will give an overview of scientific publishing, covering all the information you need to know about publishing your research. As well as providing an introduction to the Royal Society of Chemistry we will cover: how to write your paper, submission checklist, peer-review, ethics and open access – along with our editors' top tips.			
17:30	Poster session			

19:00	Close
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Tuesday 4 April 2023

09:00	PL03 PLENARY - Session Chair: Anthony Meijer Breaking the red limit: photosynthesis in far-red light Roberta Croce, VU University Amsterdam, Netherlands			
10:00	Time for delegates to move between theatres			
Theme	Understanding surface catalyst molecular interactions during catalysis	Astrochemistry and chemistry at cold temperatures	Dynamics of soft matter	Digital chemistry and machine learning
Session chair	Haresh Manyar	Wendy Brown	Carlos Avendano	J. Grant Hill
10:10	K05 KEYNOTE Enhancing emission control performance through doped ceria catalysts: insights into NOx storage, release, and reduction mechanisms Nancy Artoli, Queen's University Belfast, UK	K06 KEYNOTE Space molecules – formation, destruction and collisional excitation in the gas phase Ian Sims, University of Rennes, France	K07 KEYNOTE How do pharmaceuticals crystallize? Sarah (Sally) L Price, University College London, UK	K08 KEYNOTE Atomic-scale machine learning for inorganic materials chemistry Volker Deringer, University of Oxford, UK
10:50	USC01 Large-scale DFT simulations towards catalytic hydrogenation reactions on supported PdCx nanoparticles Apostolos Kordatos, University of Southampton, UK	AC04 Energy dependent mechanistic switching in the dissociation of the CO2 dication Patrick Robertson, University of Oxford, UK	SM04 Dynamics of driven polymer transport through a nanopore Kaikai Chen, University of Chinese Academy of Sciences, China	DC04 High-throughput virtual screening of existing organic chromophores for materials discovery Omer Omar, University of Liverpool, UK
11:10	USC02 Mechanism of photocatalytic conversion of methane to ethane on PdCu/TiO2 photocatalyst Natalia Martinsinovich, University of Sheffield, UK	AC05 Enhanced reactivity of curved PAHs towards atomic hydrogen John Thrower, Aarhus University, Denmark	SM05 Recruitment of receptors at supported lipid bilayers induced by strong and weak multivalent binding Jurriaan Huskens, University of Twente, Netherlands	DC05 A natural language processing (NLP)-based deep learning approach to predict solubility parameters for drug discovery Jiayun Pang, University of Greenwich, UK
11:30	Refreshments			
Theme	Development of fluorescent materials and techniques	Physical chemistry for net zero - towards a sustainable future	Operando and in situ applications of neutron scattering	Understanding surface catalyst molecular interactions during catalysis
Session chair	Anthony Meijer	Anabel Lanterna	Emily R. Draper	Nancy Artoli
12:00	DF01 Exploring trianguleniiums as fluorescence-based lifetime probes for G-quadruplex DNA Tigerlily Bradford, Imperial College London, UK	PC01 Efficient carboxysome inspired enzymatic carbon dioxide reduction from low concentration sources through understanding of the local environment Sam Cobb, University of Cambridge, UK	OIS01 A quasi-elastic neutron scattering (QENS) study of methanol diffusion dynamics in H-ZSM-5 as a function of Si/Al ratio Santhosh Matam, The UK Catalysis Hub and Cardiff University, UK	USC03 Structure sensitivity of Cu nanoparticles supported on manganese oxide in hydrogenation of levulinic acid Nayan Jyoti Mazumdar, Queen's University Belfast, UK
12:20	DF02 BODIPY-based red fluorescent molecular rotors for microviscosity sensing Karolina Maleckaite, State Research Institute Center for Physical Sciences and Technology, Lithuania	PC02 Moving towards closed materials cycles and a circular economy. Optimising chemical recycling processes through thermal analysis Philip Davies, Waters UK, UK	OIS02 Confined fluids studied by total neutron scattering Marta Falkowska, University of Manchester, UK	USC04 Ab initio predictions for elementary adsorption and reaction steps in catalysis by acidic zeolites - a challenge for quantum chemistry Joachim Sauer, Humboldt University Berlin, Germany
12:40	DF03 The development of fluorescent, analyte-sensitive aerogels for space applications Alex Thomas, University of Nottingham, UK	PC03 Harvesting triplet excitons and enhancing emission for photon upconversion using optical cavities Robert Gordon, University of Sheffield, UK	OIS03 Rapid hydrogen mobility over a Ru nanoparticle-doped polar MgO(111) surface Tatchamapan Yoskamtorn, University of Oxford, UK	
13:00	Lunch and posters			
14:00	RSC careers talk Careers are changing. They are no longer linear, with regular structured progression. Your working life could last for 50 years and in that time you may have multiple careers. With a particular emphasis on the wide range of career options for chemistry researchers, inside and outside of academia, this session will show you how to develop ideas for your future career and where and how to look for your next role.			
Theme	Development of new biophysical methods	New spectroscopic approaches to measuring chemical mechanisms	Rational design of soft and bio materials	Frontiers in excited state chemistry
Session chair	Neil T. Hunt	Brianna Heazlewood	Andrew Parnell	Vas Stavros
14:30	BM03 Combining spectroscopic techniques to unravel the binding of an osmium polypyridyl probe to G-quadruplex structures in solution Mark Stitch, University College Dublin, Ireland	NS02 New opportunities for ultrafast time resolved 2D-IR spectroscopy in zeolite catalysis research Paul Donaldson, STFC-UKRI, UK	RD01 Biology Exploits Geometry: Impact of Aspect Ratio on Protein Networks Matt Hughes, University of Leeds, UK	FES04 Luminescent radical molecules with addressable high-spin states: Combination of optical and spin resonance spectroscopies reveals unique mechanism Sebastian Gorgon, University of Cambridge, UK
14:50	BM04 Reconstructing complete native genome of a virus from cryo-EM density: correspondence between the measured resolution and RNA flexibility Dmitry Nerukh, Aston University, UK *Online	NS02 A time-resolved infrared spectroscopy-led mechanistic study into manganese carbonyl catalysed C-H bond functionalisation reactions Jonathan Eastwood, University of York, UK	RD02 Cationic lipidoids: protonation-driven self-assembly and membrane-targeting antimicrobial activity James Jennings, University of Graz, Austria	FES05 Probing ultrafast electronic and hydrogen dynamics with ultrafast electron diffraction and transient X-ray absorption Nanna Holmgaard List, KTH Royal Institute of Technology, Sweden

15:10	BM05 Single-molecule orientation localisation microscopy using a polarisation camera Ezra Bruggeman, University of Cambridge, UK		NS04 Photonic crystal fibre: a novel optofluidic platform for sensing and photochemistry Anita Jones, University of Edinburgh, UK		RD03 Light-responsive cubosomes: triggering molecular release with stretch-squeeze lattice control Beatrice Jones, University of Cambridge, UK	FES06 Dynamics of proton transport through time-resolved vibrational spectroscopy in a protic ionic liquid Sourav Maiti, STFC, Rutherford Appleton Laboratory, UK
15:30	BM06 Sub-millisecond translational and orientational dynamics of a freely moving single nanoprobe Joseph Beckwith, University of Cambridge, UK		NS05 Planar laser-induced fluorescence (pLIF) used to determine the dynamics of inelastic hydroxyl radical collisions with liquid surfaces Daniel Moon, Heriot-Watt University, UK		RD04 Engineering the porosity of colloidal gels via shape and patchiness Carina Karner, Technical University of Vienna, Austria	FES07 Equatorial restriction of the photo-induced Jahn-Teller switch in Mn(III)-cyclam complexes Ryan Phelps, University of Edinburgh, UK
15:50	Refreshments					
16:20	PL04 PLENARY - Session Chair: Caroline Dessent Mass spectrometry in reaction mechanism research Jana Roithová, Radboud University, Nijmegen, Netherlands					
17:20	Poster session and refreshments					
19:00	Close					
19:30	Conference dinner					

Wednesday 5 April 2023

Theme	Frontiers in excited state chemistry		Operando and in situ applications of neutron scattering		Rational design of soft and bio materials	Physical chemistry for net zero - towards a sustainable future
Session chair	Caroline Dessent		Eddie Cussen		Dwaipayan Chakrabarti	Oscar Kelly
09:00	K09 KEYNOTE Bridging the divide between ultrafast spectroscopy and next-generation skincare products and beyond Vas Stavros, University of Warwick, UK		K10 KEYNOTE Using in situ electrochemistry and SANS for self-assembling systems' Emily R. Draper, University of Glasgow, UK		K11 KEYNOTE The rational design of structural colour materials via soft matter self-assembly Andrew Parnell, University of Sheffield, UK	PC04 Machine learning for sustainable chemistry Jonathan Hirst, University of Nottingham, UK
09:20						PC05 Singlet fission occurs through intermolecular heterofission in purple bacterial photosynthetic complexes and contributes to solar energy harvesting James Pidgeon, University of Sheffield, UK
09:40	FES08 Competing proton-transfer and electron-transfer dynamics, probed by Coulomb explosion imaging Daniel Strasser, The Hebrew University of Jerusalem, Israel		OIS04 Separating the measurement of rotation and translational diffusion in a cryo-condensed molecular glass Andrew Cassidy, Aarhus University, Denmark		RD05 From monomer sequence to charge mobility in semiconductor polymers via model reduction Suryoday Prodhon, University of Liverpool, UK	K12 KEYNOTE Heterogeneous photocatalysts: hurdles and opportunities throughout the solar spectrum Anabel Lanterna, University of Nottingham, UK
10:00	FES09 Non-adiabatic electronic and vibrational ring-opening dynamics resolved with attosecond core-level spectroscopy Karl Michael Ziem, Max Planck School of Photonics, Friedrich-Schiller-University Jena, Germany		OIS05 Probing the adsorption of the organic friction modifier GMO at the iron oxide-dodecane interface in situ with neutron reflectometry Alexander Armstrong, ISIS Neutron and Muon Source, UK		RD06 Interfacial enhanced ultra-robustGel hybrids for epidermal bio-monitoring Bin Xu, University of Northumbria, UK	
10:20	Making science greener – community perspectives and solutions Science and technology are key to a more sustainable future – from clean energy technologies to tackling disease – and laboratories are essential to carrying out the research, analysis and teaching that underpin these advances. However, laboratory buildings, processes and equipment, by their nature, can be resource and energy intensive. This session will highlight some key findings from the RSC's Sustainable Labs report, share ideas and discuss the challenges and opportunities to drive forward lab sustainability in the chemical sciences. rsc.li/sustainable-labs					
10:50	Refreshments					
Theme	Digital chemistry and machine learning		Dynamics of soft matter		Photophysics of functional and solar energy materials	Measurement of molecules and reactions in complex environments
Session chair	Volker Deringer		Sarah (Sally) L Price		Martijn Zwijnenburg	Dan Stone
11:20	DC06 Teaching core-hole spectroscopy to a deep neural network Conor Rakine, University of York, UK		SM06 Translucency and temperature dependence for the slip length of water on graphene Han Li, Tsinghua University, China		K01 KEYNOTE Spectral conversion materials for luminescent solar devices Rachel Evans, University of Cambridge, UK	MM03 Developing a solvothermal reaction cell for in situ neutron scattering of crystallisation Mark Crossman, University of Warwick
11:40	DC07 Benchmarking machine-learned interatomic potentials for reactive surface dynamics at metal surfaces: accuracy vs speed Wojciech Stark, University of Warwick, UK		SM08 Computer simulations of water diffusion through thermoset polymers: Applications to corrosion protection coatings Charlie Wand, University of Exeter, UK			MM04 Ultrafast dynamics of molecular chromophores in solution Julia Weinstein, University of Sheffield, UK

12:00	<p>DC08</p> <p>Towards uncertainty quantification in deep neural networks predicting X-ray absorption spectra</p> <p>Sneha Verma, Newcastle University, UK</p>		<p>PFS05</p> <p>Excited state dynamics of Cu(I) photosensitisers with ultrafast X-ray spectroscopy</p> <p>Rory Cowin, University of Sheffield, UK</p>	
12:20	Time for delegates to move between theatres			
12:30	<p>PL05</p> <p>PLENARY - Session Chair: Caroline Dessent</p> <p>The physicochemical dynamics of exhaled aerosols and airborne disease transmission</p> <p>Jonathan Reid, University of Bristol, UK</p>			
13:30	Chairs' summary and close of meeting			
13:45	Lunch			