Nancy Artoli

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Keynote speaker

Faraday joint interest group conference 2023

3 - 5 April 2023, Sheffield, UK

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ROYAL SOCIETY OF CHEMISTRY

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 Anstöter, 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, Univeristy 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

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 Martsinovich, 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 trianguleniums 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 spectrosopy-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 Prodhan, 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 Ziems, 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-robustgGel hybrids for epidermal bio-monitoring** Bin Xu, University of Northumbria, UK	
10:20	**Making science greener – community perspectives and solutions** Science and technology and 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	**DC08** **Towards uncertainty quantification in deep neural networks predicting X-ray absorption spectra** Sneha Verma, Newcastle University, UK				**PFS05** **Excited state dynamics of Cu(I) photosensitisers with ultrafast X-ray spectroscopy** Rory Cowin, University of Sheffield, UK		
12:20	Time for delegates to move between theatres						
12:30	**PL05** **PLENARY - Session Chair: Caroline Dessent** **The physicochemical dynamics of exhaled aerosols and airborne disease transmission** Jonathan Reid, University of Bristol, UK						
13:30	**Chairs' summary and close of meeting**						
13:45	Lunch						