

**2nd Faraday Joint Interest Group Conference**  
**29-31 March 2021, online**  
**Day 1: Monday 29 March**

12.00	Welcoming remarks Anthony Meijer, University of Sheffield Conference Chair													
12.10	Plenary (Chair: Anthony Meijer, University of Sheffield) Molecular processes between the stars Ewine van Dishoeck, University of Leiden													
12.50	Break: Ask the Plenary Speaker													
Theme	Magnetic materials				Next-generation quantum chemical methods				Structure of molecules				Excited state processes	
Session chair	Eddie Cussen, University of Sheffield				Scott Habershon, University of Warwick				Micaela Matta, University of Liverpool				Tom Penfold, University of Newcastle	
13.20			Electrical detection of paramagnetic and ferromagnetic resoances in Mn-perovskite Mahendiran Ramanathan, National University of Singapore	13.20	Keynote	Correlated motion in three-body coulomb systems Hazel Cox, University of Sussex	13.20	Keynote	Non-covalent interactions in odorants Maria Sanz, King's College London	13.20	Keynote	In silico photochemical erxperiments with non-Born-Oppenheimer molecular dynamics Basile Curchod, Durham University		
13.35			Unravelling the behaviour in a TCNQ based molecular solid Adam Berlie, ISIS Neutron and Muon Source, Science and Technology Facilities Council	13.50		Efficient potential energy surfaces using multiple Hartree-Fock solutions Hugh Burton, University of Oxford	13.50		Insights into DNA aptamer structure: the effects of force-field and salt concentration Zak Hughes, University of Bradford	13.50		Understanding the controllable dynamics of Pt(II) DBA systems Heather Carson, The University of Sheffield		
13.40				14.05		A linear-scaling method for noncovalent interactions: ALMO+RPAd Grant J Hill, University of Sheffield	14.05		Understanding the role of solvation in the folding and unfolding of amphipathic helices Natasha Rhys, King's College London	14.05		BoostCrop: ultrafast time-resolved insights into light-to-heat mechanisms for crop growth Jack Woolley, University of Warwick		
14.20	Break: online networking and ice breaker session													
Theme	Magnetic materials				Next-generation quantum chemical methods				Structure of molecules				Excited state processes	
Session chair	Devashibhai Adroja, Science and Technology Facilities Council				Reinhard Maurer, University of Warwick				Natalia Martsinovich, University of Sheffield				Julia Weinstein, University of Sheffield	
15.00	Keynote		Spinon confinement in the one dimensional f-electron metal Yb2Pt2Pb William Gannon, University of Kentucky	15.00		New analysis tools for excited-state quantum chemistry: turning numbers into chemical insight Felix Plasser, Loughborough University	15.00		Probing azlene-water interactions and azulene aggregation by broadband rotational spectroscopy Shefali Saxena, King's College London	15.00		Generation of a universal probe for time resolved photoelectron spectroscopy using high harmonic generation Briony Downes-Ward, University of Southampton		
15.15				15.15	Approximations to thermal symmetric time-correlation functions Christopher Robertson, University of Warwick	15.15	Photoelectron angular distributions from resonant two-photon ionisation of adiabatically aligned naphthalene James Thompson, University of Nottingham	15.15	Probing structure-function relationships in thermally-activated delayed fluorescence emitters using electron spin resonance spectroscopy Bluebell Drummond, University of Cambridge					
15.30			The Fe19 high-spin molecular magnet: ground state, excitations and intermolecular interactions Francis Pratt, STFC	15.30		Multiscale polarisable embedding of quasiparticle and electron-hole excitations from many-body Green's functions (GW-BSE) with VOTCA-XTF Gianluca Tirimbó, Eindhoven University of Technology	15.30		DFT and QM/MM modelling of Polyoxometalates (POMs): new storage materials for future generation energy devices Emanuele Falbo, University of Newcastle	15.30		Unravelling the mechanism of excited state interligand energy transfer and the engineering of dual-emission in [Ir(C^N)2(N^N)]+ complexes Paul Elliott, University of Huddersfield		
15.45	Flash poster presentations													
16.15	Poster session													
17.15	Close of formal sessions – informal networking													

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**Day 2: Tuesday 30 March**

9.45	Poster session											
11.15				Structure of molecules		Theme	Machine learning methods in material property prediction		Theme	Excited state processes		
				Maria Sanz, King's College London		Session chair	Gabor Csanyi, University of Cambridge		Session chair	Basile Curchod, Durham University		
					Theoretical modelling of the electrochemical behaviour of the graphene / hexaaminoruthenium system Natalia Martsinovich University of Sheffield	11.15		The process for creating a general-purpose machine learned potential for silicon carbide Harry Tunstall, University of Warwick	11.15		Competition between the heavy atom effect and vibronic coupling in donor-bridge-acceptor organometallics Julien Eng, Newcastle University	
					Eumelanin: a biocompatible mixed conductor Micaela Matta University of Liverpool	11.30		An accurate and transferable machine learning potential for carbon Patrick Rowe, University College London	11.30		Investigating diketopyrrolopyrrole photochemistry: transient absorption spectroscopy and wave packet analysis Daniel Polak, University of Bristol	
11.30												
11.45												
12.00	Plenary (Chair: Jan Verlet, University of Durham) Chemical dynamics with ultrashort optical and X-ray pulses Majed Chergui, École Polytechnique Fédérale de Lausanne											
12.40	Break: Ask the Plenary Speaker											
Theme	Astrochemistry and chemistry at cold temperatures				Biophysics and imaging			Photocatalysis			Excited state processes	
Session chair	Martin McCoustra, Heriot-Watt University				Lisa-Marie Needham, University of Wisconsin-Madison			Martijn Zwijnenburg, University College London			Julia Westmayr, University of Warwick	
13.10	Keynote		Astrochemistry at the dawn of star and planet formation Paola Caselli, Max Planck Institute	13.10	Keynote	Revisiting the structure-function relationship with mass photometry Philipp Kukura, University of Oxford	13.10		Unraveling the photocatalytic potential of modified Imogolite nanotubes for hydrogen production Erwan Paineau, CNRS	13.10		Towards controlling photoreactivity with mode-specific vibrational excitation Julia Weinstein, University of Sheffield
13.40			Probing the evolution of high mass protostars: an ALMA astrochemical survey Naomi Asabre Frimpong, University of Manchester	13.40		Democratizing single-molecule FRET: open-source hardware and software for determining accurate absolute distances and equilibrium dynamics Tim Craggs, University of Sheffield	13.25	Keynote	TBC Andy Cooper, University of Liverpool	13.25		MCTDH on-the-fly: efficient grid-based quantum dynamics without pre-computed potential energy surfaces Gareth Richings, University of Warwick
13.55	Extended break: alternative career paths in chemistry Robert Bowles, Royal Society of Chemistry											
Theme	Astrochemistry and chemistry at cold temperatures				Biophysics and imaging			Photocatalysis			Machine learning methods in material property prediction	
Session chair	Terry Dillon, University of York				Steven Lee, University of Cambridge			Junwang Tang, University College London			Francesca Baletto, King's College London	
15.00	Keynote		The role of complexes and tunnelling for chemical kinetics at very cold temperatures Dwayne Heard, University of Leeds	15.00	Keynote	Mesoscopic imaging of large biomedical specimens using the Mesolens Gail McConnell, University of Strathclyde	15.00		Interactions of titania (TiO2) photocatalyst with water micropollutants: a density functional theory study Manasi R. Mulay, University of Sheffield	15.00	Keynote	Machine learned force fields Gabor Csanyi, University of Cambridge
15.30			Using FELIX to study infrared photo-desorption of CO under model interstellar conditions Wendy Brown, University of Sussex	15.30		IR spectroscopy of a mosquito: A new (and needed) method to study malaria vectors Mario Gonzalez Jimenez, University of Glasgow	15.30		Ultrafast dynamics in photocatalysis/photoelectrodes studied by femtosecond x-ray absorption spectroscopy Yohei Uemura, Paul Scherrer Institut	15.30		Further developments and applications of machine learning configuration interaction Jeremy Coe, Heriot-Watt University
15.45			Kinetics of the reactions between aromatic molecules and the CN radical at astrophysically-relevant temperatures Divita Gupta, CNRS	15.45		ThX – A next-generation probe for the early detection of amyloid aggregates Lisa-Maria Needham, University of Wisconsin-Madison	15.45		Fabrication of hybrid photocatalysts for visible light activation Natalia Sergeeva University of Leeds	15.45		Deep tensor neural network representation of the electronic structure of molecules and materials Reinhard Maurer, University of Warwick
16.00	Plenary (Chair: Sanghamitra Mukhopadhyay, Science and Technology Facilities Council) Spectroscopic and dynamical probes of alkene ozonolysis reaction pathways Marsha I. Lester, University of Pennsylvania											
16.40	Break: Ask the Plenary Speaker											
17.10	Close of formal sessions – informal networking											

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**Day 3: Wednesday 31 March**

12:00	Plenary (Chair: Andrew Masters, University of Manchester) Shaping colloidal bananas to reveal biaxial, splay-bend nematic, and smectic phases Roel Dullens, University of Oxford													
12.40	Break: Ask the Plenary Speaker													
Theme	Photophysics of functional and solar cell materials				Neutron spectroscopy and allied techniques				Soft matter and biological structures				Simulation and modelling of astrochemical and atmospheric processes	
Session chair	Olof Johansson, University of Edinburgh				Sanghamitra Mukhopadhyay, Science and Technology Facilities Council				Andrew Masters, University of Manchester				Sergio Ioppolo, Queen Mary University London	
13.10	Keynote		Energetic up/down conversion in organic semiconductors and photoactive proteins Jenny Clark, University of Sheffield	13.10	Keynote	Combining quasielastic neutron scattering and other allies: a versatile tool to tackle diverse problems Arantxa Arbe, CSIC-UPV	13.10	Keynote		Simulating the growth of bacterial biofilms: spatial structure formation and evolution Rosalind Allen, University of Edinburgh	13.10	Keynote		How to interpret molecules in space: a forward-looking view of astrochemical modelling Serena Viti, Leiden University/UCL
13.40			Energy transfer in biohybrid nanoconjugate photosystems to enhance light harvesting Giordano Amoroso, University of Bristol	13.40		SANS study of electrolyte accessibility into novel heteroatom-loaded activated carbons used for supercapacitor electrodes Mojtaba Mirzaeian, University of the West of Scotland	13.40	SMTG Early Career Prize Presentation and Lecture			13.40			Tracing shock type with chemical diagnostics: an application to L1157 Tomas James, University College London
13.55			Charge transfer states and triplets in organic photovoltaics: from small molecules to ultra-low band gap polymers Tracey Clarke, University College London	13.55		Probing IL-gas interactions with neutron scattering Leila Moura, Queens University of Belfast	13.55			Statistical mechanics of polymers with topological interactions Davide Michieletto, University of Edinburgh	13.55			Phosphorus chemistry in planetary atmospheres John Plane, University of Leeds
14.10	Extended break: publishing in RSC journals Anna Simpson, Royal Society of Chemistry													
Theme	Photophysics of functional and solar cell materials				Neutron spectroscopy and allied techniques				Soft matter and biological structures				Simulation and modelling of astrochemical and atmospheric processes	
Session chair	Tom Oliver, University of Bristol				Andrew McCluskey, European Spallation Source				Patrick Warren, STFC				Anthony Meijer, University of Sheffield	
15.15	Contributing		Watching and controlling energy transport in dense materials on nanometer scales Milan Delor, Columbia University	15.15		INS studies of the methanol-to-hydrocarbon reaction Stewart Parker, STFC Rutherford Appleton Laboratory	15.15			Reversible trapping of colloids in microgrooved channels by diffusiophoresis Guido Bolognesi, Loughborough University	15.15			Molecular line emission as a tracer of the dust-grain size distribution within AGB outflows Marie Van de Sande, KU Leuven
15.30			Radical photophysics towards efficient light-emitting diodes with doublet emission Emrys Evans, University of Cambridge	15.30		Structural changes on sorption: can host or guest provide an insight into reaction? Ian Silverwood, STFC	15.30			Social distancing in colloidal crystals: less is more Dwaipayan Chakrabarti, University of Birmingham	15.30			A novel chemical mechanism for organic aerosol precursors (HOMs) suitable for global climate modelling James Weber, Univeristy of Cambridge
15.45			Operando optical tracking of single-particle ion dynamics in batteries Christoph Schnedermann, University of Cambridge	15.45		Orientation of insulin adsorbed at interfaces determined by sum frequency generation and surface-enhanced Raman spectroscopy Heike Arnolds University of Liverpool	15.45			Mesoscale modeling of degradation and erosion of swollen polymer networks Olga Kuksenok, Clemson University	15.45			Prestellar Formation of Glycine via Dark Chemistry Sergio Ioppolo, Queen Mary University London
16.00	Plenary (Chair: Claire Vallance, University of Oxford) Proton-coupled electron transfer in catalysis and energy conversion Sharon Hammes-Schiffer, Yale University													
16.40	Break: Ask the Plenary Speaker													
17.10	Presentation of poster prizes Anna Simpson, Royal Society of Chemistry													
17.20	Closing remarks and acknowledgments Claire Vallance, University of Oxford Faraday Division President													
17.30	Close of meeting													