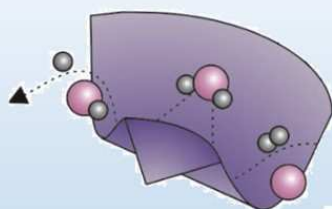


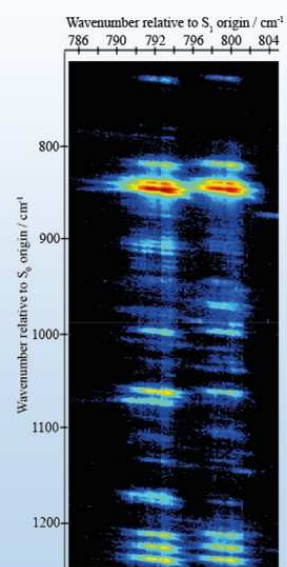
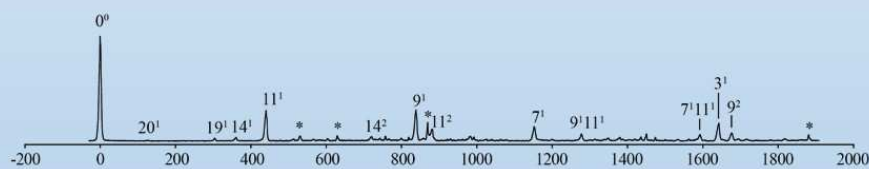
RSC Spectroscopy and Dynamics Group



University of
Nottingham
UK | CHINA | MALAYSIA



SDG 2019



University of Nottingham

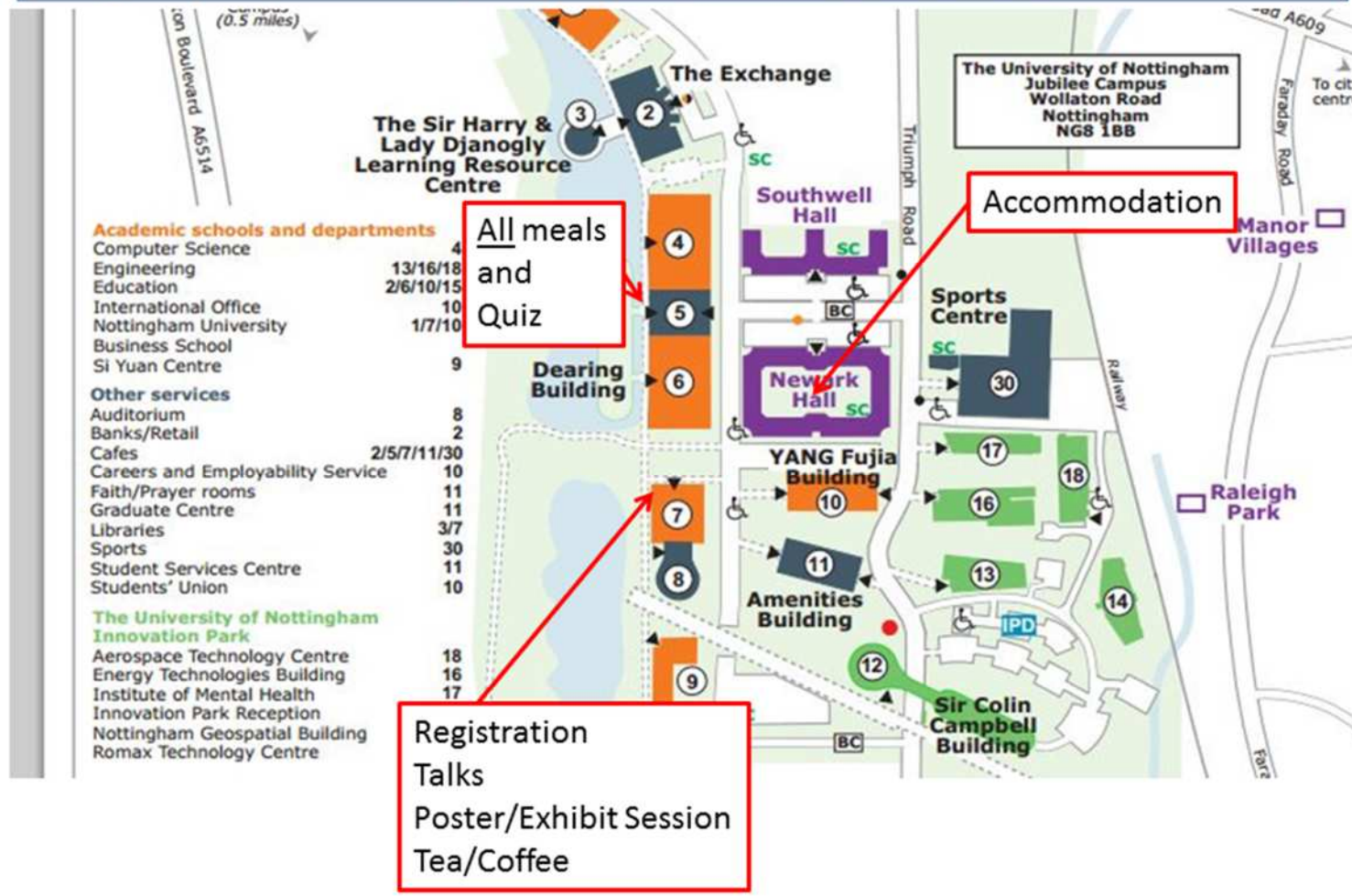


SPONSORS

As well as the Royal Society of Chemistry, we would like to thank all of our sponsors below, for their extremely generous support of this year's meeting. You are encouraged to visit them during the conference, particularly during the Poster session on Tuesday, but also during the tea and coffee breaks.



Parking is included in the conference fee for residents and day delegates. If you are a resident, you will receive your pass at Newark Hall, and you can use the parking outside of the hall. For day delegates, you can pick the passes up at the Registration desk; you can use any of the "Orange Zone" spaces. Please display the parking vouchers promptly: our parking attendants are quite vigilant! Parking is always subject to availability.



Programme

All activities will take place on the Jubilee Campus in the Business School South Building

Monday 7th January

16:00 — 18:00 **Arrival and Registration**, Newark Hall

17:30 — 19:00 **Dinner** Atrium

Session 1 Business School South Room B52

Chair: Patrick Robertson Bristol

19:10 – 19:15 **Welcome**

19:15 — 20:00 Invited Tutorial Lecture **Valerie Blanchet** Université de Bordeaux

Photoelectron spectroscopy of chiral molecules

20:00 — 20:45 Invited Tutorial Lecture **Tom Oliver** University of Bristol

Introduction to ultrafast multidimensional optical spectroscopies

Newark Hall bar is open until 23:30.

Tuesday 8th January

07:00 — 08:30 **Breakfast** Atrium

Session 2 Business School South Room B52

Chair: Matthew Frye University of Durham

08:45 — 09:30 Invited Lecture **Michael Tarbutt** Imperial University

Cooling molecules to microkelvin temperatures: methods and applications

09:30 — 09:50 Contributed Talk 1 **Alice Henley** University College London

New twists on the relaxation dynamics of the photoactive yellow protein chromophore

09:50 — 10:10 Contributed Talk 2 **Eva Gougoula** University of Newcastle

Barriers to internal rotation in methylated imidazoles by broadband rotational spectroscopy

10:10 — 10:30 Contributed Talk 3 **George Metcalfe** University of Sheffield

Real time monitoring of gases in the biosciences using FTIR and cavity-enhanced Raman spectroscopy

10:30 — 11:00 **Tea/Coffee including Trade Display (in Foyer)**

Session 3 Business School South Room B52

Chair: Tom Sharples Heriot Watt University

11:00 — 11:20 Contributed Talk 4 **Julien Eng** University of Newcastle

On the importance of intermediate states in the TADF mechanism: a matter of spin-vibronic coupling

11:20 — 11:40 Contributed Talk 5 **Elena Alonso** University of Valladolid

Microwave spectrum of vitamin B₆: the pyridoxine and pyridoxal forms

11:40 — 12:00 Contributed Talk 6 **Kasra Amini ICFO (Barcelona)**

Imaging isolated molecules with a single attosecond electron wave packet

12:00 — 12:20 Contributed Talk 7 **Rachel James** Open University

Using mid-IR and vacuum-UV spectroscopy to study interstellar ice analogues

12:20 — 12:40 Contributed Talk 8 **Alan Lewis** University of Chicago

Quantum chemistry for pump-probe spectroscopy

12:40 — 13:00 Contributed Talk 9 **Niclas West** University of Leeds

Do reaction rate coefficients reach limiting values at low temperatures?

13:00 — 14:00 **Lunch** Atrium

Session 4 Business School South Room B52

Chair: Paul Lane Heriot-Watt University

14:05 — 14:50 Invited Lecture **Heather Lewandowski** JILA, Colorado

Controlled ion-molecule reactions

14:50 — 15:10 Contributed Talk 10 **Jamie Riley** University College London

Using photoelectron spectroscopy as the solution to solvation effects on the green fluorescent protein chromophore

15:10 — 15:30 Contributed Talk 11 **Stuart Crane** University of Bristol

Wavelength-dependent ultrafast relaxation dynamics of the eumelatonin subunit 5,6-dihydroxyindole

15:30 — 15:50 Contributed Talk 12 **Ecaterina Burevschi** King's College London

Interactions of Cyclooctanone with Water: Structures and Reactivity

15:50 — 18:15 **Trade Display and Poster Session** Business School South Foyer

Including:

15:50 — 16:20 **Tea/Coffee**

17:30 — 18:30 SDG Annual General Meeting in B52

18:00 – Bar Open in the Atrium

18:45 — 20:30 **Dinner**, Atrium

20:30 — 22:30 **SDG Annual Quiz** Atrium (bar located in Atrium)

Bar open in Atrium until midnight

Wednesday 9th January

07:00 — 08:30 **Breakfast** Atrium

Session 5 Business School South Room B52

Chair: Thomas Wall Imperial College London

RSC Chemical Dynamics Award Lecture

08:45 — 09:30 Invited Lecture **Klaas Wynne** Glasgow

Delocalised phonon-like modes in biomolecules

09:30 — 09:50 Contributed Talk 13 **Aditi Bhattacharjee** University of Bristol

From ultrafast to ultraslow: watching a photoinduced catalytic cycle with a high repetition rate, mid-infrared probe

09:50 — 10:10 Contributed Talk 14 **Matt Turner** University of Warwick

Use of explicit-solvent modelling in theoretical spectroscopy

10:10 — 10:30 Contributed Talk 15 **Emily Warne** University of Southampton

Photodissociation dynamics of methyl iodide

10:30 — 11:00 **Tea/Coffee** (last chance to see posters!)

Session 6 Business School South Room B52

Chair: Adrian Gardner University of Liverpool

11:00 — 11:20 Contributed Talk 16 **Jack Woolley** University of Warwick

Photoprotective properties of mycosporine amino acids

11:20 — 11:40 Contributed Talk 17 **Joanne Woodhouse** University of Southampton

Using chemical substitutions to tune the photophysics of biological fluorophores

11:40 — 12:00 Contributed Talk 18 **James Thompson** University of Missouri

Translational energy release from laser ablation: delayed extraction time of flight mass spectrometry measurements of gadolinium plasma

12:00 — 12:20 Contributed Talk 19 **Jason Lee** University of Oxford

Combining coulomb explosion imaging and slice-imaging with the PImMS sensor

12:20 — 12:40 Contributed Talk 20 **Nikoleta Kotsina** Heriot-Watt University

Ultrafast Molecular Spectroscopy Using a Hollow-Core Photonic Crystal Fibre Light Source

12:40 — 13:00 Contributed Talk 21 **Golda Mensa-Bonsu** University of Durham

I⁻ICF₃: A frontside attack S_N2 pre-reaction complex

13:00 — 14:00 **Lunch** Atrium

Session 7 Business School South Room B52

Chair: Graham Cooper University of Bristol

14:05 — 14:50 Invited Lecture **Rachel Crespo-Otero** Queen Mary's London

Modelling effects of aggregation on excited states

14:50 — 15:10 Contributed Talk 22 **Felix Allum** University of Oxford

Imaging photodynamics using Coulomb explosion imaging and covariance analysis

15:10 — 15:30 Contributed Talk 23 **Julia Davies** University of Leicester

Infrared spectroscopy of ions originating from helium nanodroplets

15:30 — 15:50 Contributed Talk 24 **Rosaria Cercola** University of York

UV laser spectroscopy of CO-releasing molecules for pharmaceutical applications

15:50 — 16:10 Contributed Talk 25 **Maksymilian Roman** Heriot-Watt University

Making molecular movies - real-time and real-space imaging of OH collisions with liquid surfaces

16:10 **Close of Meeting** Jan Verlet

16:15 – 16:45 **Tea/Coffee and Departure**

Posters

Poster #	Presenter(s)	Institution	Poster Title
1	James Thompson	University of Missouri	Translational Energy Release from Laser Ablation: Delayed Extraction Time of Flight Mass Spectrometry measurements of Gadolinium Plasma
2	Martin Mugglestone	University of Leicester	A Theoretical Investigation into Ng-AgF (Ng = He, Ne, Ar) Complex Formation in Helium Nanodroplets
3	Marcin Konowalczyk Jessica Walton	University of Oxford	Broadband cavity-enhanced spectroscopy studies of magnetic field effects
4	Omri Tau	University College London	Time-Resolved Liquid-Microjet Photoelectron Spectroscopy
5	Jutta Toscano	University of Oxford	Making a pure beam of radicals
6	Jack Woolley	University of Warwick	Symmetric functionalisation of a UV commercial chemical filter
7	Niclas West	University of Leeds	Temperature Dependence of Collisional Energy Transfer and Reaction Rate Coefficients
8	Tomas Lock Feixas	University of York	Conformational Determination of a Flexible Molecule using Gas-Phase Electron Diffraction
9	Aditi Bhattacharjee Mahima Sneha	University of Bristol	Ultrafast Photochemical Dynamics of Organic Molecules in Solution
10	Natalie Gee Kwan Wong	University of York	Insights into the Intrinsic Absorption Properties and Photofragmentation Pathways of the Protonated Form of the Sunscreen Avobenzene
11	Kasra Amini	University of Oxford	Probing ultrafast chemical dynamics and imaging gas-phase isomers by Coulomb explosion imaging
12	Kasra Amini	ICFO-Barcelona	Imaging the Renner-Teller effect using laser-induced electron diffraction
13	Kathy Wu	University of Oxford	Using Evolutionary Algorithms to Improve Zeeman Deceleration
14	Trevor Sears	Stony Brook University	Velocity-changing collisions and broadening of sub-Doppler resonances
15	David Kemp	University of Nottingham	Vibration and torsion interactions in para-fluorotoluene via 2D-Laser Induced Fluorescence Spectroscopy
16	Anand Patel	University College London	Shining new light on firefly bioluminescence using organic synthesis and anion photoelectron spectroscopy
17	Andriana Tsikritea Lorenzo Petralia	University of Oxford	Charge exchange reaction between cold Xe ⁺ ions and ammonia isotopologues
18	Eleanor Burrow	University of York	Using hydrogen bonding as a probe of the cyclobutadiene automerization pathway in the cyclobutadiene-HF dimer
19	Natércia Rodrigues Lopes	University of Warwick	Wavepacket insights into the photoprotection mechanism of the UV filter methyl anthranilate
20	Giovanni Romanelli	STFC	Making a movie of real-life catalysed conversion of liquid and solid hydrogen
21	Divya Papat	University of Oxford	Reaction dynamics, velocity map imaging, and imaging mass spectrometry

22	Fred Cascarini Patrick Robertson	University of Bristol	An Ethane REMPI scheme in the mid-UV
23	Joe Leng	Heriot-Watt University	Stereodynamics of Inelastic Collisions of NO(A) with Atoms and Molecules
24	Graham Cooper Lingfeng Ge	University of Bristol	Simulating Coulomb Explosions
25	Felix Plasser	University of Loughborough	Boosting the efficiency of nonadiabatic dynamics simulations through vibronic coupling models
26	David Heathcote	University of Oxford	Dynamics of electron ionisation studied using velocity-map imaging
27	Paul Lane	Heriot-Watt University	Scattering dynamics of CN radicals at the gas-liquid interface
28	Cate Anstoter	University of Durham	Dipole-bound states in anions
29	Georgia Thornton Tony Kao	University of Bristol	Observing Transient Intermediates in Solution with Ultrafast Spectroscopy
30	Katya Moncrieff	Heriot-Watt University	CW-FM spectroscopy as a probe of scattering dynamics at the gas-liquid interface
31	Ryan Phelps	University of Bristol	Observing the fate of keto-carbenes using ultrafast spectroscopy
32	Sven Koehler	Manchester Metropolitan University	Characterisation, Orientation and Coverages of Functionalised Graphene by Sum-Frequency Generation Spectroscopy
33	Sam Armenta Butt	University College London	The reaction of Ar ²⁺ and O ₂ : bond forming chemistry at high potential energy
34	Alice Green Gabriele Meizyte	University of Oxford	Infrared Studies of Decorated Metal Clusters
35	Briony Downes- Ward	University of Southampton	Time-resolved XUV photoelectron spectroscopy of methyl-iodide
36	Adam Chatterley	Aarhus University	Creation and Control of Dimers in Helium Droplets
37	Aude Lietard	University of Durham	Electron attachment selectivity to a water cluster: surface vs internal binding
38	Tom Sharples	Heriot-Watt University	Spatial Separation of Methanol Clusters through Stark Deflection
39	Andre Rebelo	The Open University	Tracing reaction products to specific neutral clusters in Stark-deflected beams
40	Thomas Stonelake	University of Cardiff	Ligand Tunable Ir(III) Complexes: A Combined DFT And Transient Absorption Characterisation Methodology
41	Dhirendra Singh	University of Nottingham	Multiphoton photoelectron circular dichroism(PECD) in α -Pinene
42	Lisa Saalbach	Heriot-Watt University	Time-Resolved Photoelectron Imaging Studies of Steric Effects in Nitrobenzene Derivatives
43	Safia Hussain	King's College London	Effect of nitration on water binding to amino acid residues: rotational studies of microsolvated p-cresol and 4-methyl-2-nitrophenol
44	Nathan Watson	University of Cardiff	Criegee intermediates Derived from Hydrofluoroolefins: A Computational Study
45	Indira Murugachandran	King's College London	Structural Characterization of Limonene-Water Complexes by Rotational Spectroscopy

46	Jana Bocková	The Open University	Laser-thermally desorbed nucleoside targets for multi-photon ionization and electron attachment experiments
47	Shefali Saxena	King's College London	Probing Azulene-Water Interactions by Broadband Rotational Spectroscopy
48	Jacob Berenbeim	University of York	Mass Fragment Tasseography: A Statistical Approach to Photo-Fragment Pathway Determination for UV-Filter Oxybenzone
49	Matthew Frye	University of Durham	Progress towards forming ultracold $^2\Sigma$ CsYb molecules: Photoassociation spectroscopy, ground state potential, and predicted Feshbach resonances
50	Ali Alessa	University of Manchester	Dissociation Energies for π - π Stacked Dimers of Aromatic Hydrocarbons
51	Julia Bieniewska	Imperial College	A source of cold complex molecules for investigating parity violation
52	Emily Holt	Warwick University	Solution-phase Ultrafast Photodynamics of Two Salicylate Molecules Used in Sunscreen Formulations
53	Kelechi Uleanya	University of York	Photoexcitation of Iodide Ion-Thiouracil Clusters: Probing electron capture by a Non-Native Nucleobase
54	Felix Alum	University of Oxford	Imaging photodynamics using Coulomb explosion imaging and covariance analysis
55	Khezar Saeed	University of Liverpool	IR-Vis sum frequency generation spectroscopy of catalytic interfaces
56	Konstantina Krokidi	University of Warwick	Ultrafast dynamics of homosalate sunscreen molecule
57	Breanna Lynch	University of Durham	Photostop in a trap
58	Matt Turner	University of Warwick	Determination of secondary species through use of explicit-solvent TDDFT
59			
60			