

Programme

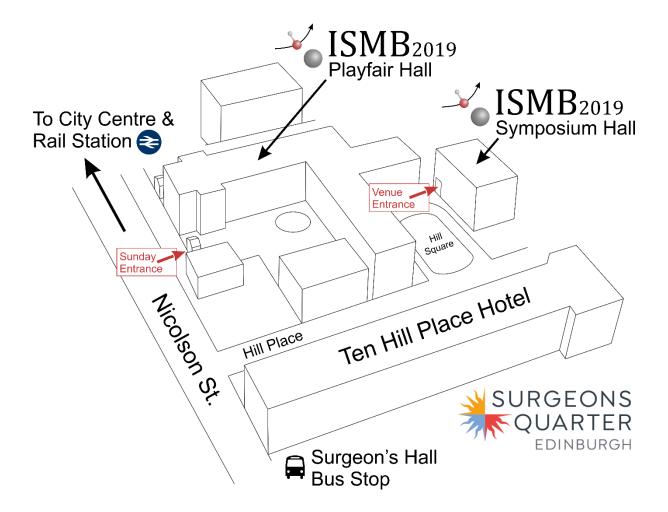
Sunday 23rd June

17:30 - 20:00 **RECEPTION**

Arrival and collection of registration materials (Playfair Hall)

Drinks and canapes will be served

All lectures and morning/afternoon session breaks will be in the Symposium Hall Reception/Drinks Reception on Sunday and both poster sessions will be held in the Playfair Hall Lunch will be in the Playfair Hall on Mon, Tues and Thurs and in the Symposium Hall on Wed and Fri WiFi Code: Since 1505



Monday 24th June

Session 1: Scattering I		Chair: Gábor Czakó (University of Szeged)			
08:45 - 09:00	Welcome and Introductory Remarks: Ken McKendrick (Heriot-Watt University)				
09:00 - 09:35	Bas van de Meerakker (Radboud University) Taming molecular collisions				
09:35 – 10:10	Mark Brouard (University of Oxford) Probing the collision mechanism via the scattering stereodynamics				
10:10 – 10:45	Nandini Mukherjee (Stanford University) Quantum control of rotationally inelastic scattering near 1 K				
10:45 – 11:15	Tea/Coffee				
11:15 – 11:50	Adam Kirrander (University of Edinburgh) Imaging molecular dynamics by ultrafast X-ray scattering				
11:50 – 12:25	Andrew Orr-Ewing (University of Bristol) Velocity map imaging of inelastic and reactive scattering dynamics				
12:25 – 12:45	HOT TOPIC: Jennifer Meyer (Universtiät Innsbruck) Indirect dynamics dominate base induced elimination (E2) for reactions of fluorine anions with tert-butyl halides				
12:45 – 14:15	Lunch (Playfair Hall)				
Session 2: F	requency-Resolved Spectroscopy	Chair: Eckart Wrede (Durham University)			
14:15 – 14:50	Anouk Rijs (Radboud University) Keep on growing: IR action spectroscopy probing peptide aggregation				
14:50 – 15:25	Scott Kable (University of New South Wales) A novel view of roaming in H_2CO from the H_2 perspective: Dividing surfaces, exit channel effects and phase space effects				
15:25 – 16:00	Cristina Puzzarini (Università di Bologna) Accurate spectroscopic characterization of molecular complexes as a first step toward understanding intermolecular interactions				
16:00 – 16:30	Tea/Coffee				
16:30 – 17:05	Maria Sanz (King's College London) Non-covalent interactions in odorants				
17:05 – 17:25	HOT TOPIC: Ulrich Bangert (University of Freiburg) Two-dimensional electronic spectroscopy of molecule				
17:30 – 19:30	Poster Session 1 (odd numbers)				

Tuesday 24th June Session 3: Time-Resolved Spectroscopy Chair: Susanne Ullrich (University of Georgia) 09:00 - 09:35Toshinori Suzuki (Kyoto University) Binding energies of solvated electrons and retrieval of true photoelectron spectra of liquids 09:35 - 10:10Baptiste Fabre (CELIA, Université de Bordeaux) Real-time monitoring of enantiomeric excess by photoelectron elliptical dichroism 10:10 - 10:45 Lionel Poisson (CNRS. Université Paris-Saclav) Self-trapping relaxation decay investigated by time-resolved photoelectron spectroscopy 10:45 - 11:15 Tea/Coffee Erik Månsson (CFEL-DESY) 11:15 - 11:50 Probing electronic processes in large molecules Jan Verlet (Durham University) 11:50 - 12:25 2D photoelectron imaging of anions as a probe of electron-driven chemistry 12:25 - 12:45 HOT TOPIC: Nikoleta Kotsina (Heriot-Watt University) Ultrafast molecular spectroscopy using a hollow-core photonic crystal fiber light source 12:45 - 14:15 Lunch (Playfair Hall + ISMB International Advisory Board meeting at 13:15 – venue TBD) Session 4: Clusters & Solvation Chair: Michal Fárník (Czech Academy of Sciences) 14:15 - 14:50 Miriam Freedman (Penn State University) Liquid-liquid phase separation in nanoscale particles Dan Neumark (University of California Berkeley) 14:50 - 15:25 Time-resolved dynamics of nucleobases in gas phase clusters and liquid water microjets 15:25 - 16:00 Ruth Signorell (ETH Zürich) Photoemission from charged droplets 16:00 - 16:30Tea/Coffee 16:30 - 17:05 Anne McCoy (University of Washington) Stories encoded in vibrational spectra: Obtaining insights into the spectroscopy of water from studies of ion-water complexes 17:05 - 17:25 HOT TOPIC: Alice Green (University of Oxford) Molecular activation and reactivity on small metal clusters

17:30 - 19:30

Poster Session 2 (even numbers)

Wednesday 26th June

Session 5: Mar	nipulation & Control	Chair: Frank Stienkemeier (University of Freiburg)			
	Jochen Küpper (CFEL-DESY and Universität Hamburg) Strong-field physics in the molecular frame toward recording the 'quantum molecular movie'				
	Brianna Heazlewood (University of Oxford) Generating a controllable beam of radicals for reaction studies				
	Henrik Stapelfeldt (Aarhus University) Laser-induced alignment and imaging of molecules embedded in helium nanodroplets				
10:45 – 11:15 Te	ea/Coffee				
	eather Lewandowski (University of Colorac ontrolled ion-radical chemistry	(0)			
	ndreas Osterwalder (École Polytechnique l old stereodynamics in merged beams	Fédérale de Lausanne)			
	OT TOPIC: Yuval Shagam (University of Control and mapping of molecular states for long coh	plorado) erence spin state readout at the quantum projection noise limit			
12:45 – 14:15 L u	unch (Symposium Hall)				

14:15 on Walking tours of historic Edinburgh (with optional whisky tasting)

14:15: Tour A (Walking & Whisky)

14:15: Tour 1 (Walking) **14:30: Tour 2** (Walking)

16:15: Tour B (Walking & Whisky)

Please arrive at Hill Square (outside Symposium Hall) <u>at least 15 mins before your designated tour departure time</u>

Thursday 27th June Session 6: Molecular Beams & Surfaces Chair: Akira Terasaki (Kyushu University) Tim Minton (Montana State University) 09:00 - 09:35Reactive-atom scattering dynamics and liquid-vacuum interfacial structure 09:35 - 10:10Daniel Farías (Universidad Autónoma de Madrid) Diffraction of CH₄ from a metal surface 10:10 - 10:45 Rainer Beck (École Polytechnique Fédérale de Lausanne) Quantum state-resolved studies of methane chemisorption and surface scattering by vibrational spectroscopies 10:45 - 11:15 Tea/Coffee Cristina Díaz (Universidad Autónoma de Madrid) 11:15 - 11:50 Exploring surface landscape with molecules: Diffraction under fast grazing incidence conditions Alec Wodtke (University of Göttingen) 11:50 - 12:25 Pump-probe experiments using pulsed molecular beams 12:25 - 12:45 HOT TOPIC: Kateryna Grygoryeva (Czech Academy of Sciences) Pyruvic acid on nanoices: Photon and electron driven chemistry 12:45 - 14:15 Lunch (Playfair Hall + Conference photo at 14:00) **Session 7: Emerging Investigator Session** Chair: Gerard Meijer (Fritz Haber Institute) 14:15 - 14:35 Bum Suk Zhao (Ulsan National Institute of Science and Technology) Scattering of aligned molecules by nonresonant optical standing waves 14:35 - 14:55 Hiroya Asami (Gakushuin University) Gas phase resonance Raman spectroscopy of huge biomolecule by IR-ablation of droplet beam: Local structure in isolated heme protein 14:55 - 15:15 Jolijn Onvlee (DESY) Unravelling the ultrafast dynamics in indole-water 15:15 - 15:45 Tea/coffee **Session 8: Honorary Session** Chair: Ken McKendrick (Heriot-Watt University) Introductory Remarks: David Chandler (Sandia National Lab) 15:45 - 16:45 David Parker (Radboud University) International Symposium on Molecular Beams: Velocity map imaging Introductory Remarks: David Nesbitt (University of Colorado) 16:45 - 17:45Marsha Lester (University of Pennsylvania) Spectroscopic and dynamical probes of atmospheric reaction pathways 18:45 on Conference Banquet (National Museum of Scotland) Drinks reception from 18:45 Dinner from 19:45

Please ensure you bring your name badge as this will be required for venue access

Friday 28th June

Session 9: Scattering II		Chair: Stuart Greaves (Heriot-Watt University)		
09:00 - 09:35	Javier Aoiz (Universidad Complutense de Madrid) Quantum stereodynamics control of inelastic and reactive collisions			
09:35 – 10:10	Arthur Suits (University of Missouri) Cold collisions of hot molecules in nearly co-propagation	agating beams		
10:10 – 10:45	Matt Costen (Heriot-Watt University) Vector and Scalar Correlations in Rotationally Inel	lastic Scattering		
10:45 – 11:15	Tea/Coffee			
11:15 – 11:50	Kopin Liu (IAMS, Academia Sinica) Benchmarking the polyatomic reaction dynamics of	of X + methane		
11:50 – 12:25	Claire Vallance (University of Oxford) Covariance-map imaging: A new tool for chemical	dynamics studies		
12:25 – 12:45	HOT TOPIC: Valentina Zhelyazkova (ETH Züric. Studying ion-molecule reactions at low temperature)			
12:45 on	Concluding Remarks & Lunch (Symposium Hal))		

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Poster Titles

- Emily Warne (University of Southampton) 1
 - Using UV and XUV time-resolved photoelectron spectroscopy to probe the dissociation dynamics of methyl iodide
- Marc Briant (CNRS, Université Paris-Saclay)

Investigation of the weak hydrogen bond of some propyne complexes

- Michal Fárník (Czech Academy of Sciences) 3
 - Electron and photon-triggered reactions between molecules adsorbed on clusters
- Ivo Vinklárek (Czech Academy of Sciences) 4

Vibrationally mediated photodissociation dynamics of pyrrole

Susanne Ullrich (University of Georgia) 5

Thionated uracils under UV irradiation: Intramolecular micro-environmental effects on the intersystem crossing dynamics

Stuart Crane (University of Bristol) 6

Coulomb explosion imaging: A tool for molecular structure determination

Aude Lietard (Durham University) 7

Localisation of the excess electron in water clusters and anthracene-water clusters

Gabriel Karras (STFC Rutherford Appleton Laboratory) 8

Following macroscopic effects in gas phase experiments using XUV-UV spectroscopy

Matija Zesko (ETH Zürich) 9

Fluorescence-lifetime-limited trapping of Rydberg helium atoms on a chip

Daniel Strasser (Hebrew University of Jerusalem) 10

Ultrafast H₃+ formation on the methanol dication: Competition of proton & electron transfer dynamics

Akira Terasaki (Kvushu University) 11

Evaporative cooling processes of liquid droplet in vacuum

Piergiorgio Casavecchia (University of Perugia) 12

Reaction dynamics of O(3P) with 1-butene and 1,2-butadiene

Gábor Czakó (University of Szeged) 13

Dynamics of bimolecular chemical reactions on ab initio potential energy surfaces

Alexandr Bogomolov (Novosibirsk State University) 14

The formation of chemically bonded argon via photoexcitation of Ar-I₂ van der Waals complex

lakov Medvedkov (Samara National Research University) 15

Design of a new molecular beams machine

Bum Suk Zhao (Ulsan National Institute of Science and Technology) 16

Matter-wave diffraction from a periodic array of half planes

Eckart Wrede (Durham University) 17

Absolute density measurements of trace amounts of OH radicals

Klaudia Gawlas (University College London) 18

Rydberg state electric field ionisation dynamics for quantum state-selective detection of resonant energy transfer in cold He* + NH3 collisions

Donatella Loru (DESY) 19

Unravelling the formation of substituted polycyclic aromatic hydrocarbons in the interstellar medium by plasma sources

Thomas Luxford (Czech Academy of Sciences) 20

Dissociative electron attachment of hydrated biomolecules

Björn Bastian (Universität Innsbruck) 21

Imaging anion-neutral reactions: Carbon chain growth and single solvent effects

Julia Bieniewska (Imperial College London) 22

Mid-infrared spectroscopy of polyatomic molecules in a cryogenic buffer gas cell and progress towards a molecular beam of cold complex molecules

Bruno Credidio (École Polytechnique Fédérale de Lausanne) 23

Gas-liquid scattering dynamics in crossed beams

Adam Deller (University College London) 24

Long-lived high Rydberg states of NO for Stark deceleration and trapping

Liam Duffy (UNC Greensboro) 25

Sub-THz cavity enhanced absorption and dispersion effects in molecular beams

Gerard Meijer (Fritz-Haber-Institut der Max-Planck-Gesellschaft) 26

Spectroscopic characterization of AIF with relevance to laser cooling and trapping

- 27 Roland Wester (Universität Innsbruck)
 Spectator behavior, enhancement, and suppression of ion-molecule reactions by vibrational excitation
- 28 Ozan Lacinbala (Institut des Sciences Moléculaires d'Orsay)
 Laboratory astrophysics: Towards a better understanding of the aromatic infrared emission features
- 29 Ondrej Votava (Czech Academy of Sciences)
 Gold-mining the molecular overtone spectra using supersonic beam techniques
- Theofanis Kitsopoulos (Georg August University and University of Crete)
 Kinetics and dynamics of CO oxidation on atomically stepped Pd surfaces
- 31 **Felix Allum** (University of Oxford)
 High-resolution sliced velocity-map imaging following newton sphere inversion
- 32 Christian Mangeng (University of Basel) Long-term trapping of Stark-decelerated polar molecules
- Tobias Sixt (University of Freiburg)
 Quantum-state-controlled Penning collisions between lithium atoms and metastable helium atoms
- 34 **Lisa Saalbach** (Heriot-Watt University)
 Time-resolved photoelectron imaging studies of steric effects in nitrobenzene derivatives
- 35 **Viktor Tajti** (University of Szeged)
 Accurate ab initio thermochemistry, potential energy surface, and dynamics of the F⁻ + CH₃CH₂Cl reaction
- Pedro Recio (University of Perugia)
 Crossed molecular beam studies of the reaction dynamics of O(3P) with 1,3-Butadiene
- Thomas Giesen (University of Kassel)
 Infrared cavity ringdown spectroscopy of molecules in supersonic jets
- 38 Paul Lane (Heriot-Watt University)
 Scattering dynamics at the gas-liquid interface
- 39 **Marco Flock** (*University of Wuerzburg*)
 A ps time-resolved photoelectron study on the photophysics of tolane
- Tibor Győri (University of Szeged)
 Automated potential energy surface development: Application to the F⁻ + CH₃Br system
- 41 Florian Hirsch (University of Wuerzburg)
 The gas-phase IR spectra of xylyl radicals
- Jochen Küpper (DESY and Universität Hamburg)
 Creating, imaging, and controlling chiral molecules with electric fields
- 43 Simon Hofsäss (*Fritz Haber Insitute*)
 Towards laser cooling and trapping of AIF molecules
- 44 Ardita Kilaj (University of Basel)
 Reaction kinetics of trapped molecular ions with conformer- and isomer-selected neutral molecules
- 45 **Domonkos Tasi** (University of Szeged) Rethinking fundamental S_N2 reactions
- Siwen Wang (University of Science and Technology of China)
 A new crossed molecular beams apparatus
- 47 Clément Soulié (Heriot-Watt University)
 Theoretical studies of electronic quenching via molecular collisions
- 48 Charlotte Jansen (Leiden University)
 Unravelling the contribution of steps to D2 dissociation on Ni(711)
- Dóra Papp (University of Szeged)
 Benchmark ab initio study of the X + C₂H₆ [X = F, Cl, Br, I] systems, dynamics of the X + C₂H₆ [X = F, Cl] reactions, and PESs for spectroscopy
- 50 Patrik Straňák (University of Basel) Investigating conformational and state-specific effects in chemical reactions
- 51 **Akihiro Kitazaki** (Gakushuin University)
 Gas phase CD spectroscopy of albumin ion in DUV region by using IR-laser ablation of droplet beam: Analysis of secondary structure
- 52 **Jolijn Onvlee** (DESY)
 Pure and aligned (bio)molecular samples
- 53 **Cornelia Heid** (*University of Oxford*)
 Comparison of spin-orbit excitations in side-on collisions of Ar with NO

Matin Kaufmann (University of Kassel) Building-up of a precision spectrometer using a REMPI detection scheme Maksymilian Roman (Heriot-Watt University) 55 Real-space imaging of OD collisions with liquid surfaces Thuy Dung Tran (Charles University) 56 Reaction of O- with H2, D2 and HD at low temperature Aggeliki Afentaki / Peter Samartzis (Foundation for Research and Technology-Hellas) 57 Multiphoton Rydberg and valence dynamics of highly excited small molecules Tom Sharples (Heriot-Watt University) 58 A change of scene: Atom-diatom scattering in an electronically excited state David Chandler (Sandia National Laboratory) 59 Two-colour alignment and dissociation of molecular hydrogen when under intense laser fields Katharina Höveler (ETH Zürich) 60 Merged molecular beams to study ion-molecule reactions at temperatures down to 300 mK Joe Leng (Heriot-Watt University) 61 Stereodynamics of the inelastic collisions of NO(A) with molecules Floriane Grollau (CNRS, Université Paris-Saclay) 62 Spectroscopy of 4(5)-methylimidazole and its hydrates, hosted in helium droplets Stuart Greaves (Heriot-Watt University) 63 Studying gas-liquid surface reactions using velocity map imaging Arthur Suits (University of Missouri) 64 UF-CRDS: A pulsed uniform flow apparatus with cw-cavity ringdown spectroscopy Bernadette Broderick (University of Missouri) 65 Product branching and low temperature reaction kinetics by chirped-pulse Fourier transform mm-wave spectroscopy in a uniform supersonic flow Hendrik Nahler (Heriot-Watt University) 66 Absolute fluorescence quantum yield of acetone Jacqueline Arlt (Aarhus Universty) 67 Molecular frame photoelectron angular distributions of aniline obtained via weak-field ionization Katya Moncrieff (Heriot-Watt University) 68 Mid-infrared frequency modulated spectroscopy as a probe of scattering dynamics at the gas-liquid interface Yuval Shagam (University of Colorado) 69* Control and mapping of molecular states for long coherence spin state readout at the quantum projection noise limit Alice Green (University of Oxford) 70* Molecular activation and reactivity on small metal clusters Kateryna Grygoryeva (Czech Academy of Sciences) 71* Pyruvic acid on nanoices: Photon and electron driven chemistry Nikoleta Kotsina (Heriot-Watt University) 72* Ultrafast molecular spectroscopy using a hollow-core photonic crystal fiber light source Bum Suk Zhao (Ulsan National Institute of Science and Technology) 73* Scattering of aligned molecules by nonresonant optical standing waves Hiroya Asami (Gakushuin University) 74* Gas phase resonance Raman spectroscopy of huge biomolecule by IR-ablation of droplet beam: Local structure in isolated heme protein Joliin Onvlee (DESY) 75* Unravelling the ultrafast dynamics in indole-water **Ulrich Bangert** (University of Freiburg) Two-dimensional electronic spectroscopy of molecules in helium nanodroplet isolation Jennifer Meyer (Universtiät Innsbruck) Indirect dynamics dominate base induced elimination (E2) for reactions of fluorine anions with tert-butyl halides Valentina Zhelyazkova (ETH Zürich) 78* Studying ion-molecule reactions at low temperatures with a merged-beam set-up

Posters denoted * also feature as either Hot Topic or Emerging Investigator talks.

		Monday 24 th June	Tuesday 25 th June	Wednesday 26 th June	Thursday 27 th June	Friday 28 th June
	08:45 - 09:00	Welcome & Introduction				
		Scattering I Chair: Gábor Czakó	Time-Resolved Spectroscopy Chair: Susanne Ullrich	Manipulation & Control Chair: Frank Stienkemeier	Molecular Beams & Surfaces Chair: Akira Terasaki	Scattering II Chair: Stuart Greaves
	09:00 - 09:35	Bas van de Meerakker	Toshinori Suzuki	Jochen Küpper	Tim Minton	Javier Aoiz
	09:35 - 10:10	Mark Brouard	Baptiste Fabre	Brianna Heazlewood	Daniel Farías	Arthur Suits
	10:10 - 10:45	Nandini Mukherjee	Lionel Poisson	Henrik Stapelfeldt	Rainer Beck	Matt Costen
	10:45 - 11:15	Coffee	Coffee	Coffee	Coffee	Coffee
	11:15 - 11:50	Adam Kirrander	Erik Månsson	Heather Lewandowski	Cristina Díaz	Kopin Liu
	11:50 – 12:25	Andrew Orr-Ewing	Jan Verlet	Andreas Osterwalder	Alec Wodtke	Claire Vallance
	12:25 – 12:45	Jennifer Meyer	Nikoleta Kotsina	Yuval Shagam	Kateryna Grygoryeva	Valentina Zhelyazkova
	12:45 – 14:15	Lunch	Lunch (IAB meeting @ 13:15)	Lunch	Lunch (Conference photo @ 14:00)	Concluding Remarks & Lunch
		Frequency-Resolved Spectroscopy Chair: Eckart Wrede	Clusters & Solvation Chair: Michal Fárník		Emerging Investigators Chair: Gerard Meijer	
	14:15 – 14:50	Anouk Rijs	Miriam Freedman	Walking tour of historic	Bum Suk Zhao	14:15 – 14:35
	14:50 – 15:25	Scott Kable	Dan Neumark	Edinburgh with optional	Hiroya Asami	14:35 – 14:55
	15:25 – 16:00	Cristina Puzzarini	Ruth Signorell	whisky tasting 14:15: Tour A (Walking & Whisky) 14:15: Tour 1 (Walking) 14:30: Tour 2 (Walking) 16:15: Tour B (Walking & Whisky)	Jolijn Onvlee	14:55 – 15:15
	16:00 – 16:30	Coffee	Coffee		Coffee	15:15 – 15:45
	16:30 – 17:05	Maria Sanz	Anne McCoy		Honorary Session	
Sunday 23 rd June	17:05 – 17:25	Ulrich Bangert	Alice Green		Chair: Ken McKendrick	
Registration & Drinks Reception	17:30 – 19:30	Poster Session 1 (Odd Numbers)	Poster Session 2 (Even Numbers)		David Parker (Introduced by David Chandler)	15:45 – 16:45
					Marsha Lester (Introduced by David Nesbitt)	16:45 – 17:45
All lectures and morning/afternoon session breaks will be in the Symposium Hall Registration/Drinks Reception on Sunday and both poster sessions will be held in the Playfair Hall Lunch will be in the Playfair Hall on Monday, Tuesday and Thursday and in the Symposium Hall on Wednesday and Friday					Conference Banquet National Museum of Scotland	Drinks: 18:45 Dinner: 19:45