HERIOT WATT UNIVERSITY

ISMB2019

XXVIIIth International Symposium on Molecular Beams

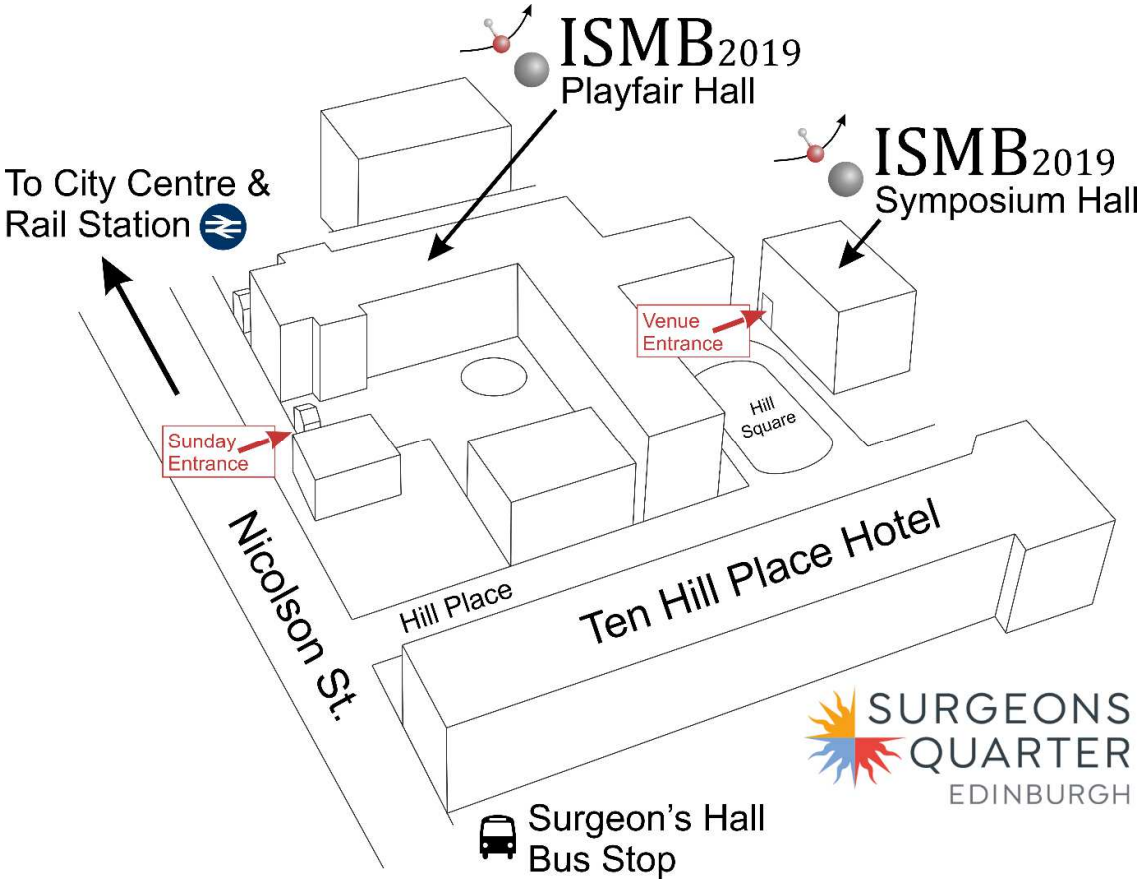
Edinburgh, Scotland
23rd - 28th June 2019

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



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	**Xueming Yang** *(Dalian Institute of Chemical Physics)* Probing geometric effects in chemical reaction
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: Frequency-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 molecules in helium nanodroplet isolation
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 – 09:35	**Toshinori Suzuki** *(Kyoto University)* Binding energies of solvated electrons and retrieval of true photoelectron spectra of liquids
09:35 – 10:10	**Baptiste Fabre** *(CELIA, Université de Bordeaux)* Real-time monitoring of enantiomeric excess by photoelectron elliptical dichroism
10:10 – 10:45	**Lionel Poisson** *(CNRS, Université Paris-Saclay)* Self-trapping relaxation decay investigated by time-resolved photoelectron spectroscopy
10:45 – 11:15	**Tea/Coffee**
11:15 – 11:50	**Erik Månsson** *(CFEL-DESY)* Probing electronic processes in large molecules
11:50 – 12:25	**Jan Verlet** *(Durham University)* 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 in Symposium Hall at 13:00)

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
14:50 – 15:25	**Dan Neumark** *(University of California Berkeley)* 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 – 16:30	**Tea/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: Manipulation & Control

Chair: Frank Stienkemeier *(University of Freiburg)*

09:00 – 09:35	**Jochen Küpper** *(CFEL-DESY and Universität Hamburg)* Strong-field physics in the molecular frame toward recording the 'quantum molecular movie'
09:35 – 10:10	**Brianna Heazlewood** *(University of Oxford)* Generating a controllable beam of radicals for reaction studies
10:10 – 10:45	**Henrik Stapelfeldt** *(Aarhus University)* Laser-induced alignment and imaging of molecules embedded in helium nanodroplets
10:45 – 11:15	**Tea/Coffee**
11:15 – 11:50	**Heather Lewandowski** *(University of Colorado)* Controlled ion-radical chemistry
11:50 – 12:25	**Andreas Osterwalder** *(École Polytechnique Fédérale de Lausanne)* Cold stereodynamics in merged beams
12:25 – 12:45	**HOT TOPIC: Yuval Shagam** *(University of Colorado)* Control and mapping of molecular states for long coherence spin state readout at the quantum projection noise limit
12:45 – 14:15	**Lunch** (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) *at least 15 mins before your designated tour departure time*

Thursday 27th June

Session 6: Molecular Beams & Surfaces

Chair: Akira Terasaki *(Kyushu University)*

09:00 – 09:35 **Tim Minton** *(Montana State University)*
Reactive-atom scattering dynamics and liquid-vacuum interfacial structure

09:35 – 10:10 **Daniel Farías** *(Universidad Autónoma de Madrid)*
Diffraction of CH_4 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**

11:15 – 11:50 **Cristina Díaz** *(Universidad Autónoma de Madrid)*
Exploring surface landscape with molecules: Diffraction under fast grazing incidence conditions

11:50 – 12:25 **Alec Wodtke** *(University of Göttingen)*
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)*

15:45 – 16:45 **Introductory Remarks:** David Chandler *(Sandia National Lab)*

David Parker *(Radboud University)*
International Symposium on Molecular Beams: Velocity map imaging

16:45 – 17:45 **Introductory Remarks:** David Nesbitt *(University of Colorado)*

Marsha 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

Friday 28th June

Session 9: Scattering II

Chair: Matt Costen *(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-propagating beams
10:10 – 10:45	**Andrew Orr-Ewing** *(University of Bristol)* Velocity map imaging of inelastic and reactive scattering dynamics
10:45 – 11:15	**Tea/Coffee**
11:15 – 11:50	**Kopin Liu** *(IAMS, Academia Sinica)* Benchmarking the polyatomic reaction dynamics 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 Zürich)* Studying ion-molecule reactions at low temperatures with a merged-beam set-up
12:45 on	**Concluding Remarks & Lunch** (Symposium Hall)

IMSB SPONSORS

Poster Titles

1	**Emily Warne** *(University of Southampton)* Using UV and XUV time-resolved photoelectron spectroscopy to probe the dissociation dynamics of methyl iodide
2	**Marc Briant** *(CNRS, Université Paris-Saclay)* Investigation of the weak hydrogen bond of some propyne complexes
3	**Michal Fárník** *(Czech Academy of Sciences)* Electron and photon-triggered reactions between molecules adsorbed on clusters
4	**Ivo Vinklárek** *(Czech Academy of Sciences)* Vibrationally mediated photodissociation dynamics of pyrrole
5	**Susanne Ullrich** *(University of Georgia)* Thionated uracils under UV irradiation: Intramolecular micro-environmental effects on the intersystem crossing dynamics
6	**Stuart Crane** *(University of Bristol)* Coulomb explosion imaging: A tool for molecular structure determination
7	**Aude Lietard** *(Durham University)* Localisation of the excess electron in water clusters and anthracene-water clusters
8	**Gabriel Karras** *(STFC Rutherford Appleton Laboratory)* Following macroscopic effects in gas phase experiments using XUV–UV spectroscopy
9	**Matija Zesko** *(ETH Zürich)* Fluorescence-lifetime-limited trapping of Rydberg helium atoms on a chip
10	**Daniel Strasser** *(Hebrew University of Jerusalem)* Ultrafast H_3^+ formation on the methanol dication: Competition of proton & electron transfer dynamics
11	**Akira Terasaki** *(Kyushu University)* Evaporative cooling processes of liquid droplet in vacuum
12	**Piergiorgio Casavecchia** *(University of Perugia)* Reaction dynamics of O(^{3}P) with 1-butene and 1,2-butadiene
13	**Gábor Czakó** *(University of Szeged)* Dynamics of bimolecular chemical reactions on ab initio potential energy surfaces
14	**Alexandr Bogomolov** *(Novosibirsk State University)* The formation of chemically bonded argon via photoexcitation of Ar-I_2 van der Waals complex
15	**Iakov Medvedkov** *(Samara National Research University)* Design of a new molecular beams machine
16	**Bum Suk Zhao** *(Ulsan National Institute of Science and Technology)* Matter-wave diffraction from a periodic array of half planes
17	**Eckart Wrede** *(Durham University)* Absolute density measurements of trace amounts of OH radicals
18	**Klaudia Gawlas** *(University College London)* Rydberg state electric field ionisation dynamics for quantum state-selective detection of resonant energy transfer in cold He* + NH_3 collisions
19	**Donatella Loru** *(DESY)* Unravelling the formation of substituted polycyclic aromatic hydrocarbons in the interstellar medium by plasma sources
20	**Thomas Luxford** *(Czech Academy of Sciences)* Dissociative electron attachment of hydrated biomolecules
21	**Björn Bastian** *(Universität Innsbruck)* Imaging anion-neutral reactions: Carbon chain growth and single solvent effects
22	**Julia Bieniewska** *(Imperial College London)* Mid-infrared spectroscopy of polyatomic molecules in a cryogenic buffer gas cell and progress towards a molecular beam of cold complex molecules
23	**Bruno Credidio** *(École Polytechnique Fédérale de Lausanne)* Gas-liquid scattering dynamics in crossed beams
24	**Adam Deller** *(University College London)* Long-lived high Rydberg states of NO for Stark deceleration and trapping
25	**Liam Duffy** *(UNC Greensboro)* Sub-THz cavity enhanced absorption and dispersion effects in molecular beams
26	**Gerard Meijer** *(Fritz-Haber-Institut der Max-Planck-Gesellschaft)* Spectroscopic characterization of AlF 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
30	**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
33	**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 $F^- + CH_3CH_2Cl$ reaction
36	**Pedro Recio** *(University of Perugia)* Crossed molecular beam studies of the reaction dynamics of $O(^3P)$ with 1,3-Butadiene
37	**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
40	**Tibor Győri** *(University of Szeged)* Automated potential energy surface development: Application to the $F^- + CH_3Br$ system
41	**Florian Hirsch** *(University of Wuerzburg)* The gas-phase IR spectra of xylyl radicals
42	**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 AlF 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
46	**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)
49	**Dóra Papp** *(University of Szeged)* Benchmark *ab initio* study of the $X + C_2H_6$ [X = F, Cl, Br, I] systems, dynamics of the $X + C_2H_6$ [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

54	**Matin Kaufmann** *(University of Kassel)* Building-up of a precision spectrometer using a REMPI detection scheme
55	**Maksymilian Roman** *(Heriot-Watt University)* Real-space imaging of OD collisions with liquid surfaces
56	**Thuy Dung Tran** *(Charles University)* Reaction of O^- with H_2, D_2 and HD at low temperature
57	**Aggeliki Afentaki / Peter Samartzis** *(Foundation for Research and Technology-Hellas)* Multiphoton Rydberg and valence dynamics of highly excited small molecules
58	**Joe Leng** *(Heriot-Watt University)* Stereodynamics of the inelastic collisions of NO(A) with molecules
59	**David Chandler** *(Sandia National Laboratory)* Two-colour alignment and dissociation of molecular hydrogen when under intense laser fields
60	**Katharina Höveler** *(ETH Zürich)* Merged molecular beams to study ion-molecule reactions at temperatures down to 300 mK
61	**Tom Sharples** *(Heriot-Watt University)* A change of scene: Atom-diatom scattering in an electronically excited state
62	**Floriane Grollau** *(CNRS, Université Paris-Saclay)* Spectroscopy of 4(5)-methylimidazole and its hydrates, hosted in helium droplets
63	**Stuart Greaves** *(Heriot-Watt University)* Studying gas-liquid surface reactions using velocity map imaging
64	**Arthur Suits** *(University of Missouri)* UF-CRDS: A pulsed uniform flow apparatus with cw-cavity ringdown spectroscopy
65	**Bernadette Broderick** *(University of Missouri)* Product branching and low temperature reaction kinetics by chirped-pulse Fourier transform mm-wave spectroscopy in a uniform supersonic flow
66	**Hendrik Nahler** *(Heriot-Watt University)* Absolute fluorescence quantum yield of acetone
67	**Jacqueline Arlt** *(Aarhus University)* Molecular frame photoelectron angular distributions of aniline obtained via weak-field ionization
68	**Katya Moncrieff** *(Heriot-Watt University)* Mid-infrared frequency modulated spectroscopy as a probe of scattering dynamics at the gas-liquid interface
69*	**Yuval Shagam** *(University of Colorado)* Control and mapping of molecular states for long coherence spin state readout at the quantum projection noise limit
70*	**Alice Green** *(University of Oxford)* Molecular activation and reactivity on small metal clusters
71*	**Kateryna Grygoryeva** *(Czech Academy of Sciences)* Pyruvic acid on nanoices: Photon and electron driven chemistry
72*	**Nikoleta Kotsina** *(Heriot-Watt University)* Ultrafast molecular spectroscopy using a hollow-core photonic crystal fiber light source
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74*	**Hiroya Asami** *(Gakushuin University)* Gas phase resonance Raman spectroscopy of huge biomolecule by IR-ablation of droplet beam: Local structure in isolated heme protein
75*	**Jolijn Onvlee** (DESY) Unravelling the ultrafast dynamics in indole-water
76*	**Ulrich Bangert** *(University of Freiburg)* Two-dimensional electronic spectroscopy of molecules in helium nanodroplet isolation
77*	**Jennifer Meyer** *(Universtiät Innsbruck)* Indirect dynamics dominate base induced elimination (E2) for reactions of fluorine anions with tert-butyl halides
78*	**Valentina Zhelyazkova** *(ETH Zürich)* 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 24th June	Tuesday 25th June	Wednesday 26th June	Thursday 27th June	Friday 28th 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: Matt Costen
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	Andrew Orr-Ewing
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	Xueming Yang	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 @ 13:00)	Lunch	Lunch (Conference photo @ 14:00)	Concluding Remarks & Lunch
	Frequency-Resolved Spectroscopy Chair: Eckart Wrede	***Clusters & Solvation*** Chair: Michal Fárník	**Walking tour of historic Edinburgh with optional whisky tasting**	***Emerging Investigators*** Chair: Gerard Meijer	
14:15 – 14:50	Anouk Rijs	Miriam Freedman		Bum Suk Zhao	14:15 – 14:35
14:50 – 15:25	Scott Kable	Dan Neumark		Hiroya Asami	14:35 – 14:55
15:25 – 16:00	Cristina Puzzarini	Ruth Signorell		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*** Chair: Ken McKendrick	
Sunday 23rd June 17:05 – 17:25	Ulrich Bangert	Alice Green			
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
				Conference Banquet National Museum of Scotland	Drinks: 18:45 Dinner: 19:45

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