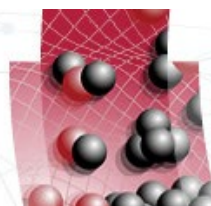


# New Directions in Molecular Scattering

8-10 May 2024 | Edinburgh, UK



Faraday  
Discussions

Wednesday 8 May 2024

11:30	Registration with lunch served from 11.45
12:45	<b>Welcome and introductions</b> Kenneth McKendrick, <i>Chair of Scientific Committee</i>
12:55	<b>Outline of Discussion format</b> Brian Li and Hugh Ryan, <i>Royal Society of Chemistry Publishing Editors</i>
13:00	<b>Introductory Lecture – Spiers Memorial Lecture</b> (Session chair: Kenneth McKendrick) Alec Wodtke <i>University of Göttingen and Max Planck Institute, Germany</i>
14:00	Comfort break (no refreshments)
	<b>Session 1</b> (Session chairs: Brianna Heazlewood & Claire Vallance)
14:15	<b>Reaction interferometry with ultracold molecules</b> Kang-Kuen Ni <i>Harvard University, US</i>
14:20	<b>Temperature dependent stereodynamics in surface scattering measured through subtle changes in the molecular wave function</b> Helen Chadwick <i>Swansea University, UK</i>
14:25	<b>Isomeric and rotational effects in the chemi-ionisation of 1,2-dibromoethene with metastable neon atoms</b> Stefan Willitsch <i>University of Basel, Switzerland</i>
14:30	<b>Determination of collision mechanisms at low energies using four-vector correlations</b> Pablo Jambrina <i>University of Salamanca, Spain</i>
14:35	Discussion
16:00	Refreshments
16:30	<b>To form or not to form a reaction complex: Exploring ion-molecule reactions between C<sub>3</sub>H<sub>4</sub> isomers and Xe<sup>+</sup> and O<sub>2</sub><sup>+</sup></b> Heather Lewandowski <i>University of Colorado, UK</i>
16:35	<b>Transient IR Spectroscopy of Optically Centrifuged CO<sub>2</sub> (R186–R282) and Collision Dynamics for the J=244–282 States</b> Amy Mullin <i>University of Maryland, US</i>
16:40	<b>Diffractive mirrors for neutral-atom matter-wave optics</b> Bum Suk Zhao <i>Ulsan National Institute of Science and Technology, South Korea</i>
16:45	Discussion
18:00	<b>Lightning presentations (by invitation of the Scientific Committee)</b> Session chair: Claire Vallance
18:15	<b>Poster session and wine reception</b> Poster judges: Helen Chadwick, Daniel Harding, Bin Jiang
19:45	Close

Thursday 9 May 2024

	<b>Session 2</b> (Session chairs: Hua Guo & Dave Chandler)
09:00	<b>Scattering resonances in the rotational excitation of HDO by Ne and <i>normal</i>-H<sub>2</sub>: theory and experiment</b> Astrid Bergeat <i>University of Bordeaux, France</i>
09:05	<b>Mixed Quantum/Classical Theory (MQCT) Approach to the Dynamics of Molecule-Molecule Collisions in Complex Systems</b> Dmitri Babikov <i>Marquette University, US</i>
09:10	<b>Vibrational energy transfer in ammonia-helium collisions</b> Jérôme Loreau <i>Katholieke University, Belgium</i>
09:15	Discussion
10:20	Refreshments
10:50	<b>Bimolecular Collision Outcomes on Multidimensional Potential Energy Surfaces: Infrared Spectroscopy and Activation of NO-Alkane Collision Complexes</b> Nathanael Kidwell <i>College of William &amp; Mary, US</i>
10:55	<b>Inelastic Scattering of NO(A<sup>2</sup>Σ<sup>+</sup>) + CO<sub>2</sub>; Rotation-Rotation Pair-Correlated Differential Cross Sections</b> Matthew Costen <i>Heriot-Watt University, UK</i>
11:00	<b>Dynamics of collisions and uptake of alcohol molecules with hydrated nitric acid clusters</b> Michal Farnik <i>The Czech Academy of Sciences, Czech Republic</i>
11:05	Discussion
12:10	Lunch
	<b>Session 3</b> (Session chairs: Rainer Beck & Hua Guo)
13:00	<b>Probing the Interfacial Structure of Aqueous Surfactants through Helium Atom Evaporation</b> Gil Nathanson <i>University Wisconsin-Madison, US</i>
13:05	<b>Dissociative chemisorption of O<sub>2</sub> on Al(111): Dynamics on a potential energy surface computed with a non-self-consistent screened hybrid density functional approach</b> Geert-Jan Kroes <i>University of Leiden, Netherlands</i>
13:10	<b>Molecular Beam Scattering of Ammonia from a Dodecane Flat Liquid Jet</b> Daniel Neumark <i>University of California, Berkeley</i>
13:15	<b>Time-Resolved Surface Reaction Kinetics in the Pressure Gap</b> Daniel Harding <i>KTH Royal Institute of Technology, Sweden</i>
13:20	Discussion
14:45	Refreshments
15:15	<b>Identification of reaction intermediates in the decomposition of formic acid on Pd</b>

	Jan Fingerhut <i>Georg-August University of Goettingen, Germany</i>
15:20	<b>On-Surface Chemical Dynamics of Monolayer, Bilayer, and Many-Layered Graphene Surfaces Probed with Supersonic Beam Scattering and STM Imaging</b> Steven Sibener <i>University of Chicago, US</i>
15:25	<b>Abortive reaction leads to selective adsorbate rotation</b> Gilbert Walker <i>University of Toronto, Canada</i>
15:30	<b>Six-dimensional Quantum Dynamics of an Eley-Rideal Reaction between Gaseous and Adsorbed Hydrogen Atoms on Cu(111)</b> Bin Jiang <i>USTC Hefei, China</i>
15:35	Discussion
17:00	Close of sessions
18:30	Pre-dinner drinks
19:00	Conference dinner – Stratosphere, Dynamic Earth

Friday 10 May 2024

	<b>Session 4</b> (Session chairs: Dave Chandler & Brianna Heazlewood)
09:00	<b>Exploring the chemical dynamics of phenanthrene (C<sub>14</sub>H<sub>10</sub>) formation via the bimolecular gas-phase reaction of the phenylethynyl radical (C<sub>6</sub>H<sub>5</sub>CC) with benzene (C<sub>6</sub>H<sub>6</sub>)</b> Ralf-Ingo Kaiser <i>University of Hawai'i at Mānoa, US</i>
09:05	<b>Crossed molecular beam experiments and theoretical simulations on the multichannel reaction of toluene with atomic oxygen</b> Nadia Balucani <i>University of Perugia, Italy</i>
09:10	<b>Reaction dynamics of S(<sup>3</sup>P) with 1,3-butadiene and isoprene: Crossed beam scattering, low temperature flow experiments, and high-level electronic structure calculations</b> Arthur Suits <i>University of Missouri, US</i>
09:15	Discussion
10:30	Refreshments
11:00	<b>Reaction Dynamics of the Methoxy Anion CH<sub>3</sub>O<sup>-</sup> with Methyl Iodide CH<sub>3</sub>I</b> Roland Wester <i>University of Innsbruck, Austria</i>
11:05	<b>Dynamics of carbene formation in the reaction of methane with the tantalum cation in the gas phase</b> Jennifer Meyer <i>University of Kaiserslautern-Landau, Germany</i>
11:10	<b>High-level analytical potential-energy-surface-based dynamics of the OH<sup>-</sup> + CH<sub>3</sub>CH<sub>2</sub>Cl SN2 and E2 reactions in full (24) dimensions</b> Gábor Czakó <i>University of Szeged, Hungary</i>
11:15	Discussion
12:30	<b>Concluding Remarks Lecture</b> (Session chair: Kenneth McKendrick) ) Mark Brouard <i>University of Oxford, UK</i>
13:00	<b>Acknowledgements and presentation of poster prizes</b>
13:15	<b>Close of meeting and lunch</b>