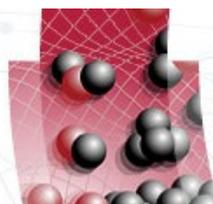


# New Directions in Molecular Scattering

8-10 May 2024 | Edinburgh, UK



Faraday  
Discussions

Wednesday 8 May 2024

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| 11:30 | Registration with lunch served from 11.45  |
| 12:45 | <b>Welcome and introductions</b><br>Kenneth McKendrick, <i>Chair of Scientific Committee</i>   |
| 12:55 | <b>Outline of Discussion format</b><br>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)<br>Alec Wodtke<br><i>University of Göttingen and Max Planck Institute, Germany</i>   |
| 14:00 | Comfort break (no refreshments)  |
|       | <b>Session 1</b><br>(Session chairs: Brianna Heazlewood & Claire Vallance)   |
| 14:15 | <b>Reaction interferometry with ultracold molecules</b><br>Kang-Kuen Ni<br><i>Harvard University, US</i>   |
| 14:20 | <b>Temperature dependent stereodynamics in surface scattering measured through subtle changes in the molecular wave function</b><br>Helen Chadwick<br><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><br>Stefan Willitsch<br><i>University of Basel, Switzerland</i>  |
| 14:30 | <b>Determination of collision mechanisms at low energies using four-vector correlations</b><br>Pablo Jambrina<br><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><br>Heather Lewandowski<br><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><br>Amy Mullin<br><i>University of Maryland, US</i>  |
| 16:40 | <b>Diffractive mirrors for neutral-atom matter-wave optics</b><br>Bum Suk Zhao<br><i>Ulsan National Institute of Science and Technology, South Korea</i>   |
| 16:45 | Discussion   |
| 18:00 | Lightning presentations (by invitation of the Scientific Committee)<br>Session chair: Claire Vallance  |
| 18:15 | Poster session and wine reception<br>Poster judges: Helen Chadwick, Daniel Harding, Bin Jiang  |
| 19:45 | Close  |

Thursday 9 May 2024

| <b>Session 2</b><br>(Session chairs: Hua Guo & Dave Chandler) |  |
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| 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><br>Astrid Bergeat<br><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><br>Dmitri Babikov<br><i>Marquette University, US</i>  |
| 09:10   | <b>Vibrational energy transfer in ammonia-helium collisions</b><br>Jérôme Loreau<br><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><br>Nathanael Kidwell<br><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><br>Matthew Costen<br><i>Heriot-Watt University, UK</i>   |
| 11:00   | <b>Dynamics of collisions and uptake of alcohol molecules with hydrated nitric acid clusters</b><br>Michal Farnik<br><i>The Czech Academy of Sciences, Czech Republic</i>  |
| 11:05   | Discussion   |
| 12:10   | Lunch  |
| <b>Session 3</b><br>(Session chairs: Rainer Beck & Hua Guo)   |  |
| 13:00   | <b>Probing the Interfacial Structure of Aqueous Surfactants through Helium Atom Evaporation</b><br>Gil Nathanson<br><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><br>Geert-Jan Kroes<br><i>University of Leiden, Netherlands</i> |
| 13:10   | <b>Molecular Beam Scattering of Ammonia from a Dodecane Flat Liquid Jet</b><br>Daniel Neumark<br><i>University of California, Berkeley</i>   |
| 13:15   | <b>Time-Resolved Surface Reaction Kinetics in the Pressure Gap</b><br>Daniel Harding<br><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>  |

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|       | Jan Fingerhut<br><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><br>Steven Sibener<br><i>University of Chicago, US</i> |
| 15:25 | <b>Abortive reaction leads to selective adsorbate rotation</b><br>Gilbert Walker<br><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><br>Bin Jiang<br><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

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|       | <b>Session 4</b><br>(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><br>Ralf-Ingo Kaiser<br><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><br>Nadia Balucani<br><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><br>Arthur Suits<br><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><br>Roland Wester<br><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><br>Jennifer Meyer<br><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 SN<sub>2</sub> and E<sub>2</sub> reactions in full (24) dimensions</b><br>Gábor Czakó<br><i>University of Szeged, Hungary</i>   |
| 11:15 | Discussion  |
| 12:30 | <b>Concluding Remarks Lecture</b> (Session chair: Kenneth McKendrick )<br>Mark Brouard<br><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>   |