

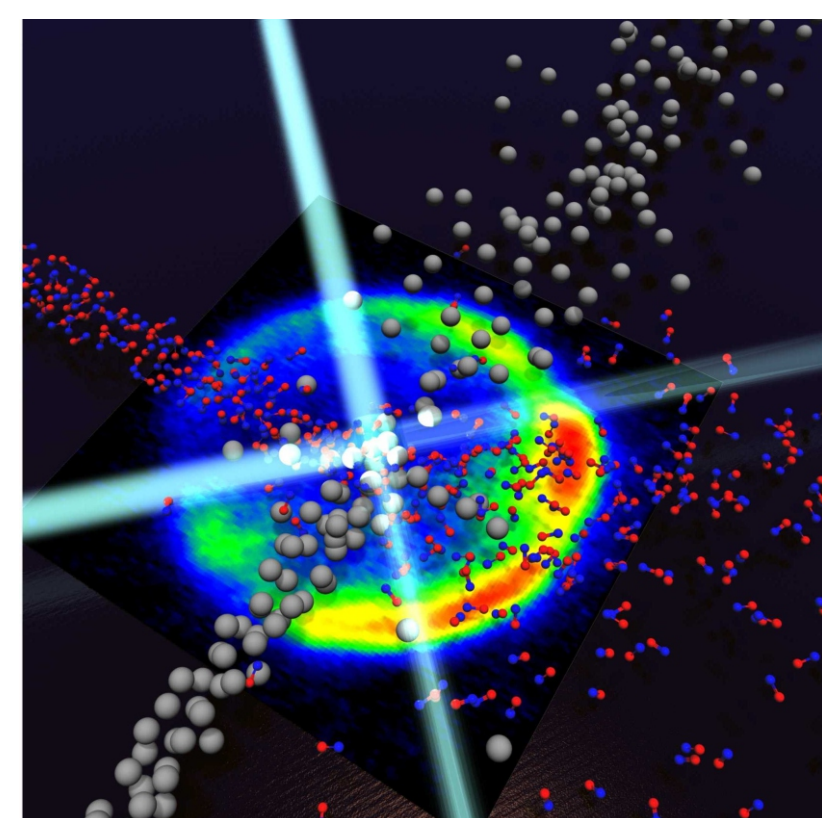


The Brouard Group

Professor Mark Brouard, Dr Cornelia Heid, Dr Felicia Green, Robert Mason, Felix Allum, Natasha Smith, Joe Mcmanus.



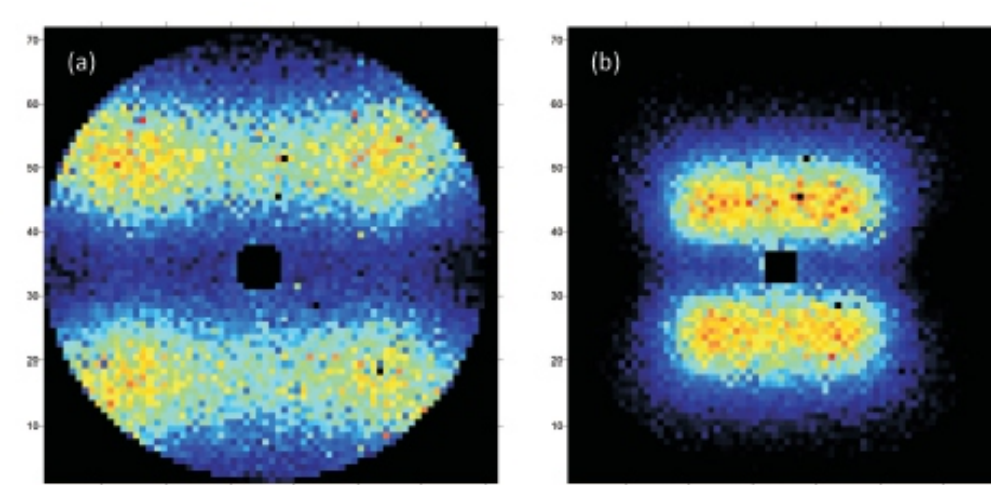
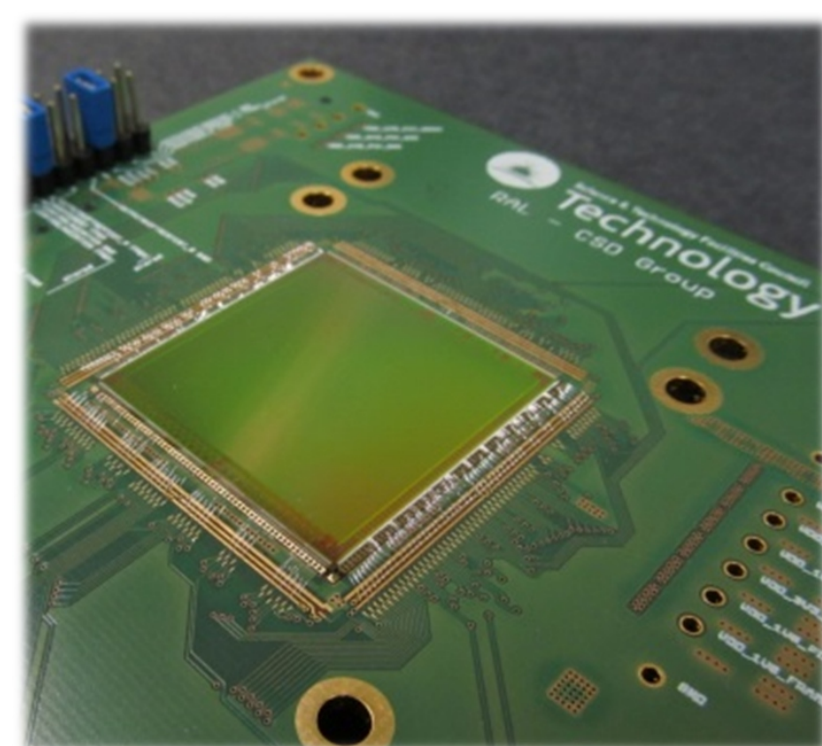
A Brief Overview



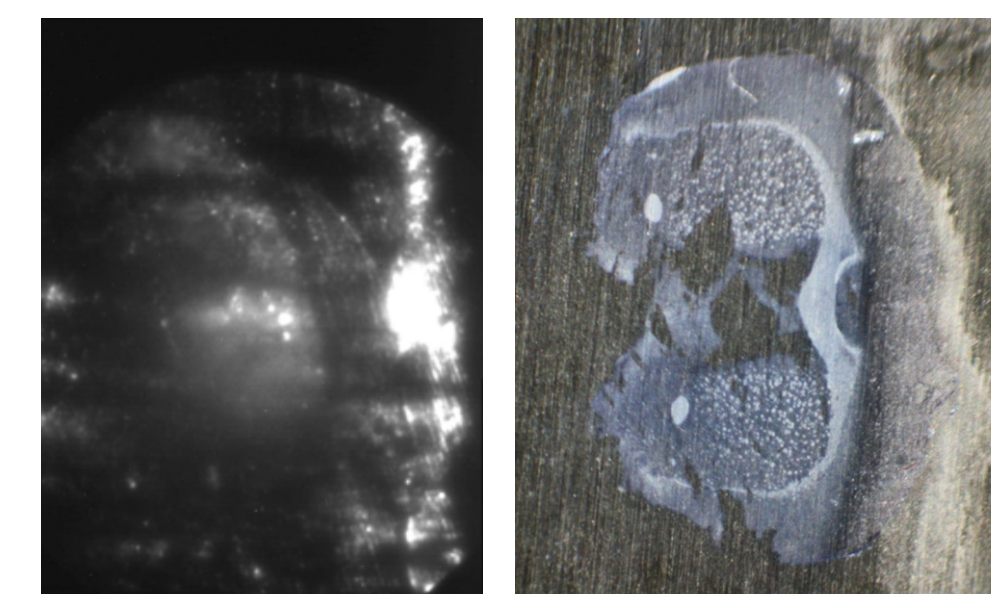
• Investigations into the dynamics of gas phase chemical processes and collisions using ion imaging techniques.

• Simulations and development of models to describe these fundamental processes.

• Development and application of chemical imaging techniques used in medical sciences, and for high throughput chemical analysis.

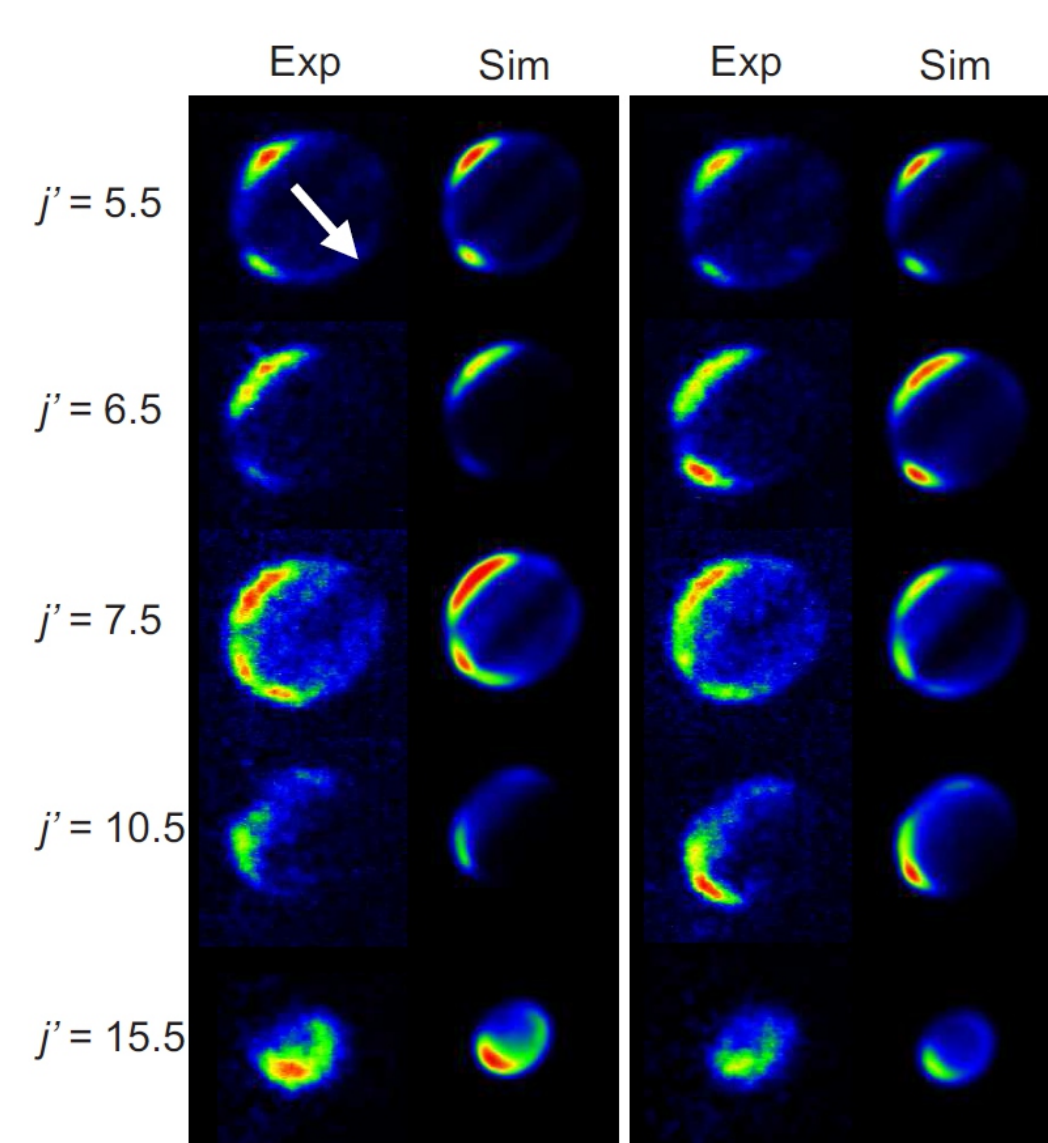


Raw ion images of the Br⁺ and F⁺ ion fragments following the Coulomb explosion of the DBrDFCyBPh molecule.

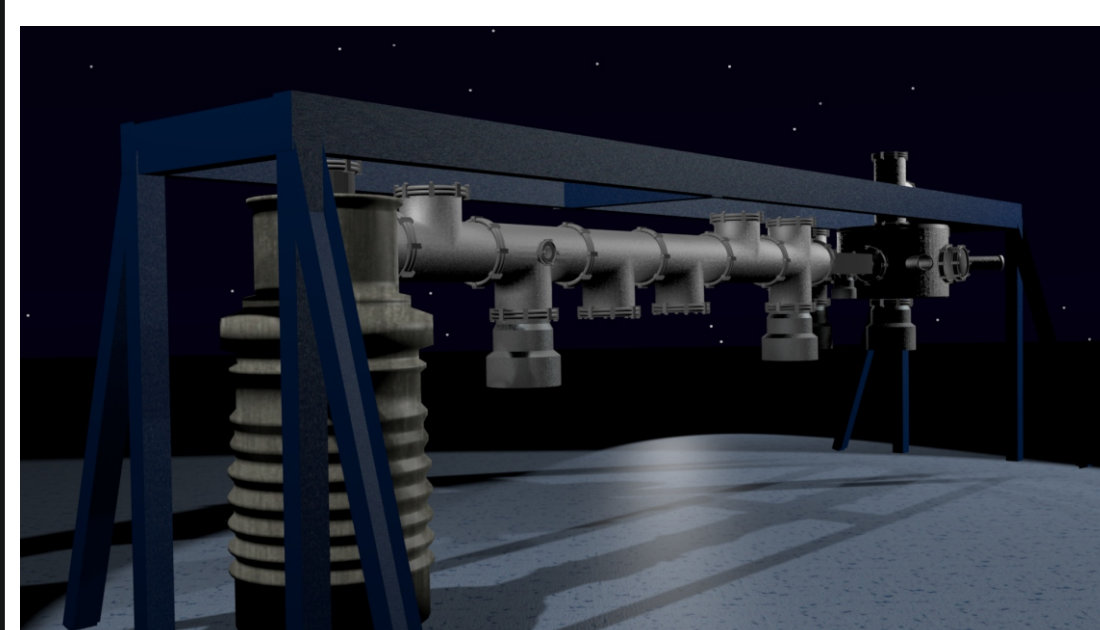


An ion (left) and optical (right) image of a biological sample.

Quantum State-Resolved Scattering



Ion images for oriented scattering of NO with Ar. The intensity reflects the state-to-state differential cross section for the collision.



Our hexapole experiment - known affectionately as the 'Blue Monster'

• The Blue Monster allows observation of the angular distribution of fully quantum state-selected scattered molecules.

• A hexapole electric field selects the initial quantum state of the NO molecules in the primary beam.

• The beam of NO molecules is then intersected by the secondary beam containing a rare gas.

• The NO can be orientated using electric fields in the scattering chamber, to produce N-end, O-end, or side-on collisions.

• The scattered NO molecules are state-selectively excited, ionised and accelerated onto a detector to give the images shown here.

• For simple systems, such as NO + rare gas, the experimental differential cross sections can be compared with high level quantum mechanical scattering calculations. The combination of our quantum state-resolved experiments with theory reveals details about the underlying quantum mechanics of such scattering processes.

• We plan to study more complex systems in the future such as NO + diatomics by changing the gas in the secondary beam.

Ultrafast Photoinduced Dynamics

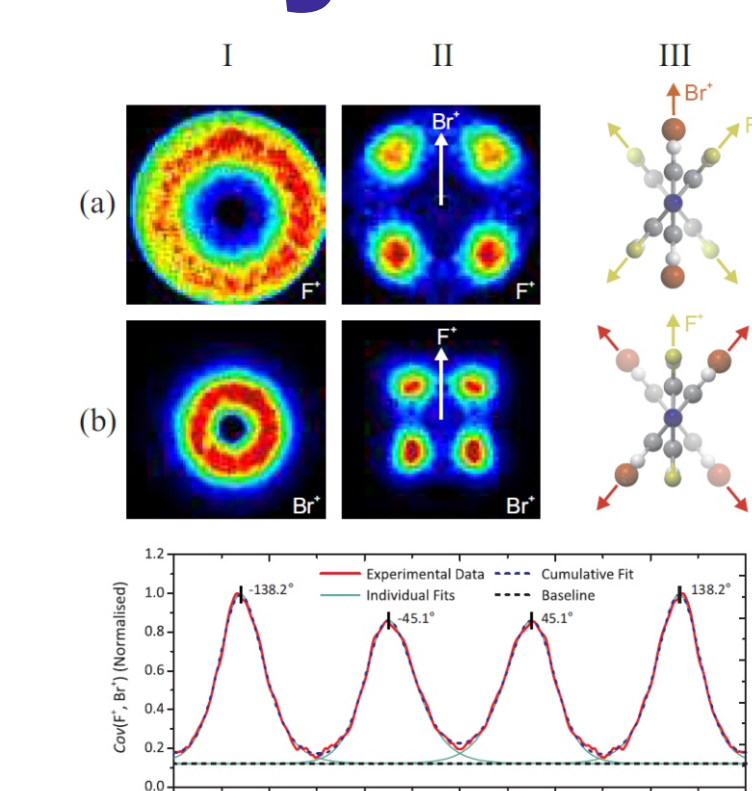
• Imaging multiple fragments from a single chemical event in coincidence can reveal detailed information about the underlying dynamics, by determining the relative momenta of different ion fragments.

• Intense femtosecond laser pulses are used to rapidly ionize target molecules, which rapidly break up into repelling charged fragments - a Coulomb explosion

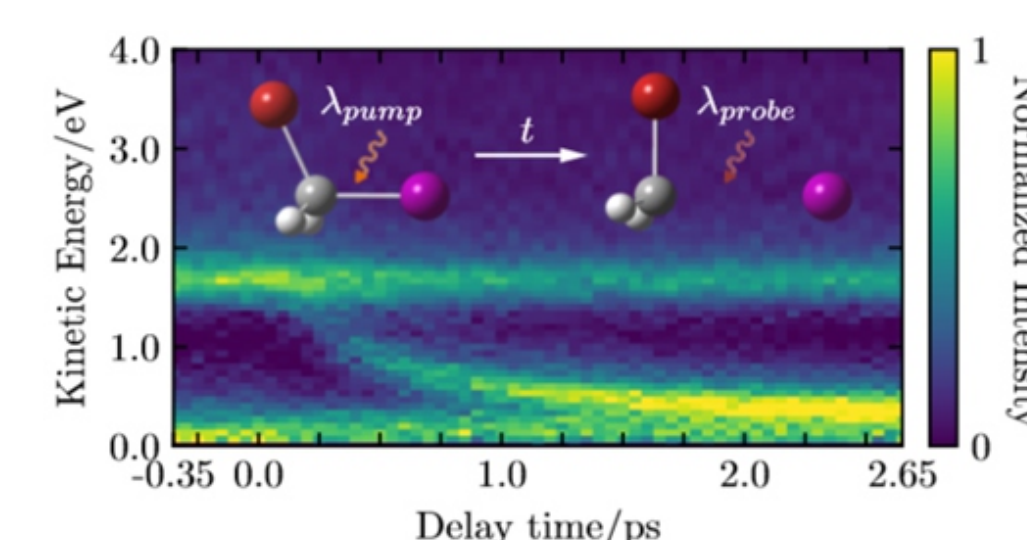
• By correlating the velocities of the resulting fragments using a technique called covariance mapping - we are able to 'probe' the system and obtain structural information about the parent molecule on a femtosecond timescale

• Preceding the intense 'probe' pulse with a 'pump' pulse to initiate some photochemistry, we are able to study the structural dynamics of such processes on a femtosecond timescale.

• Recently, we have used this technique to study a range of chemical and physical processes in real time, such as: vibrational motion, photodissociation, photoisomerisation, and charge transfer



Covariance imaging fragments from a Coulomb explosion of a substituted biphenyl molecule, allowing us to measure the dihedral angle on a femtosecond timescale

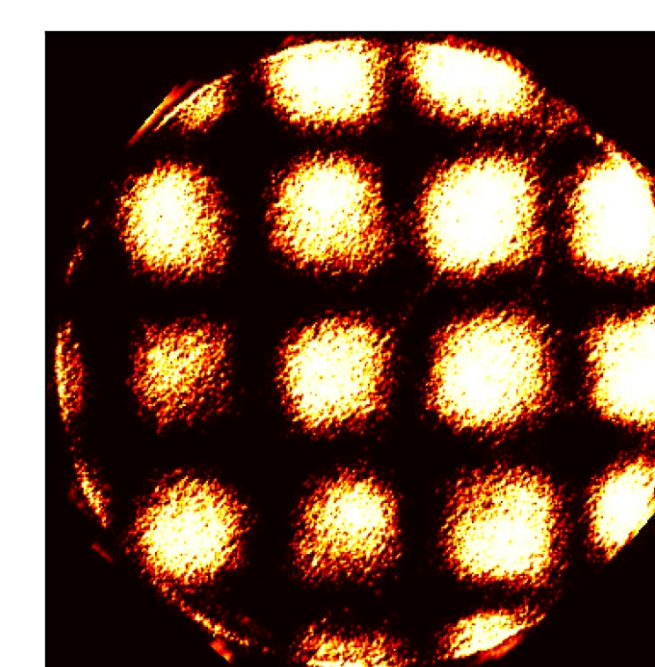


The time-resolved kinetic energy of I⁺ ions originating from the photodissociation then Coulomb explosion of CH₂BrI. The measured kinetic energy decreases as pump-probe delay increases, due to the increased charge separation at the point of Coulomb explosion

Imaging Mass Spectrometry

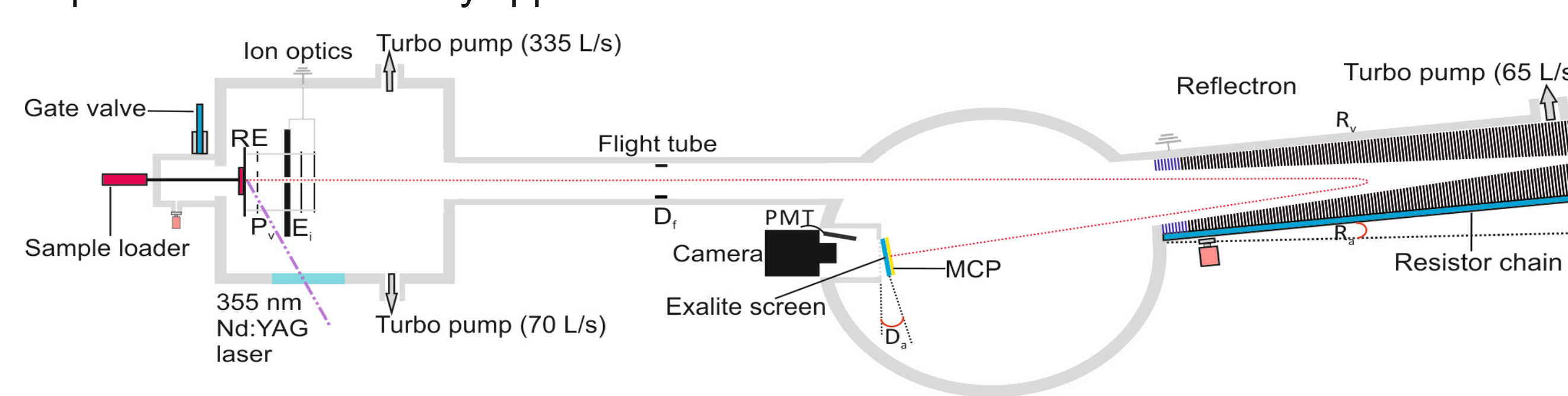
• By applying specific voltages to an ion optics assembly, we are able to image spatial distributions of ions originating from a surface irradiated by laser light.

• This allows us to create a chemical map of a surface, which has many potential application in biology and medicine. For instance, it can be used to determine where certain biomarker molecules are located in a tissue sample.



Experimental ion image showing the spatial distributions of ions at a surface

• Recent work has focussed on developing instrumentation to push the resolution limits of microscope mode mass spectrometry in the spatial and mass domains. A novel microscope-mode reflectron instrument has been developed, shown schematically below. This, in addition to new pulsed extraction schemes has greatly improved the resolution at which we can image, and the m/z range the technique can be successfully applied to.



PImMS



Pixel Imaging Mass Spectrometry

• The PImMS camera is a novel fast imaging sensor, developed in collaboration between research groups in Oxford Chemistry, Oxford Physics, and the Rutherford Appleton Laboratory (RAL).

• The camera is capable of recording ion images with a timing precision of 12.5ns, in effect combining the experimental techniques of ion-imaging and mass spectrometry.

• This allows for species of different masses to be imaged simultaneously in a single ion-imaging experiment. Traditionally, the cameras used in ion-imaging are unable to record any timing information, and so the detector system is gated to only image one ion per experimental cycle.

• The multi-mass imaging capabilities of the PImMS camera underpins the group's work in imaging mass spectrometry and photoinduced dynamics.

For further information, contact mark.brouard@chem.ox.ac.uk;

or just speak to one of the group members here - we will be happy to show you around our lab!

Angular Momentum - It makes the world go round!

