



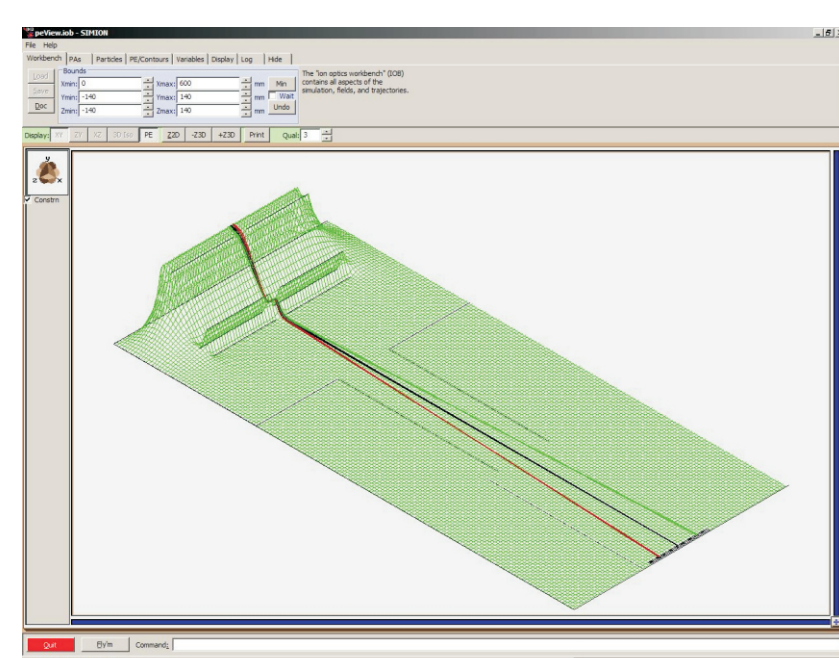
# The Brouard Group

Professor Mark Brouard, Helen Chadwick, Ed Halford, Balazs Hornung, John Lawlor, Bethan Nichols, Tom Perkins, Scott Seamons, Michael Scott, Craig Slater, Wei Hao Yuen, and Benjamin Winter



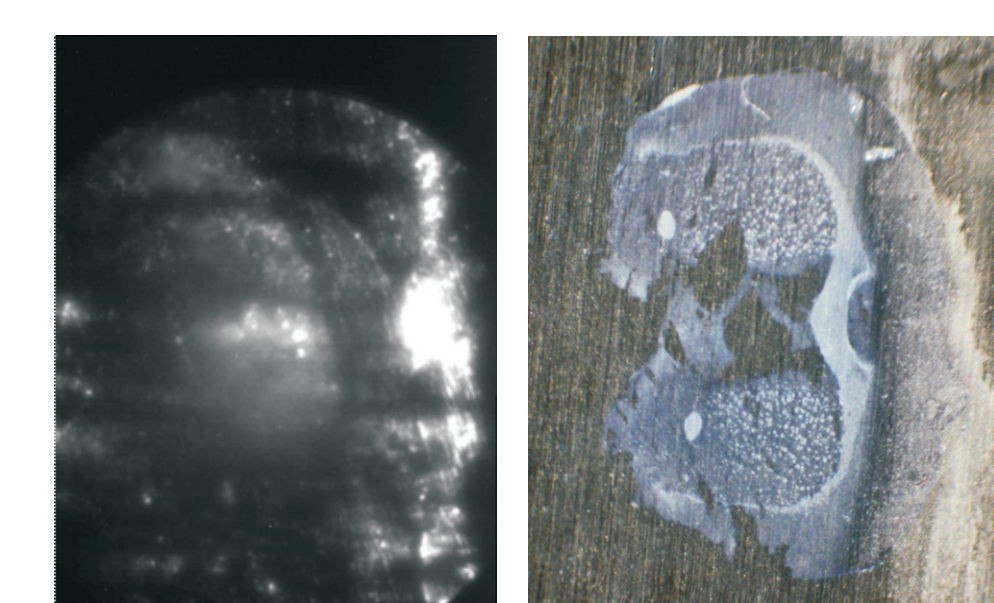
## What we do:

• Investigations into the dynamics of gas phase chemical processes and collisions using techniques such as ion imaging, and laser induced fluorescence;



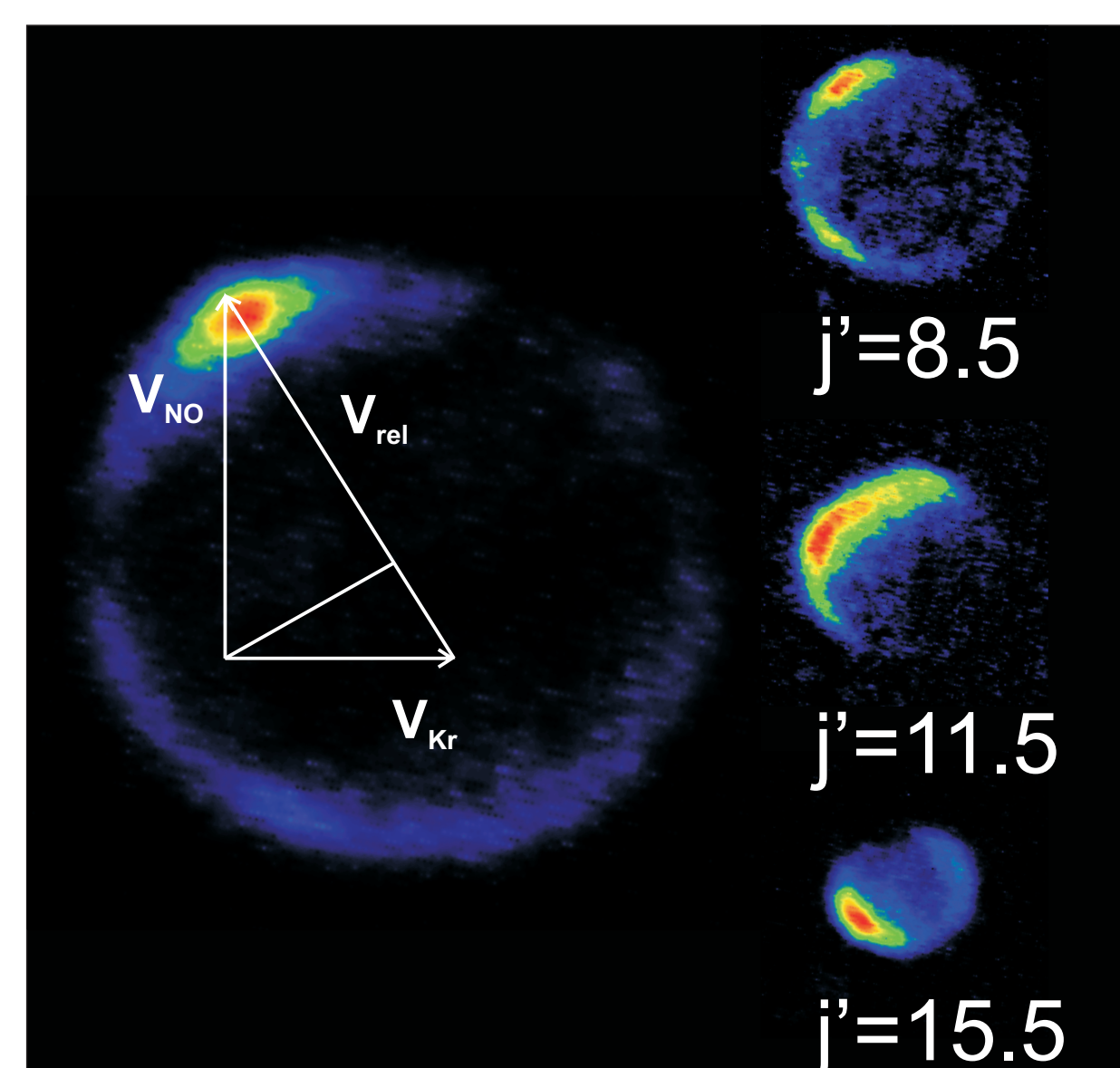
• Simulations, and the development of models used to describe these fundamental processes;

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



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

## Quantum state resolved scattering

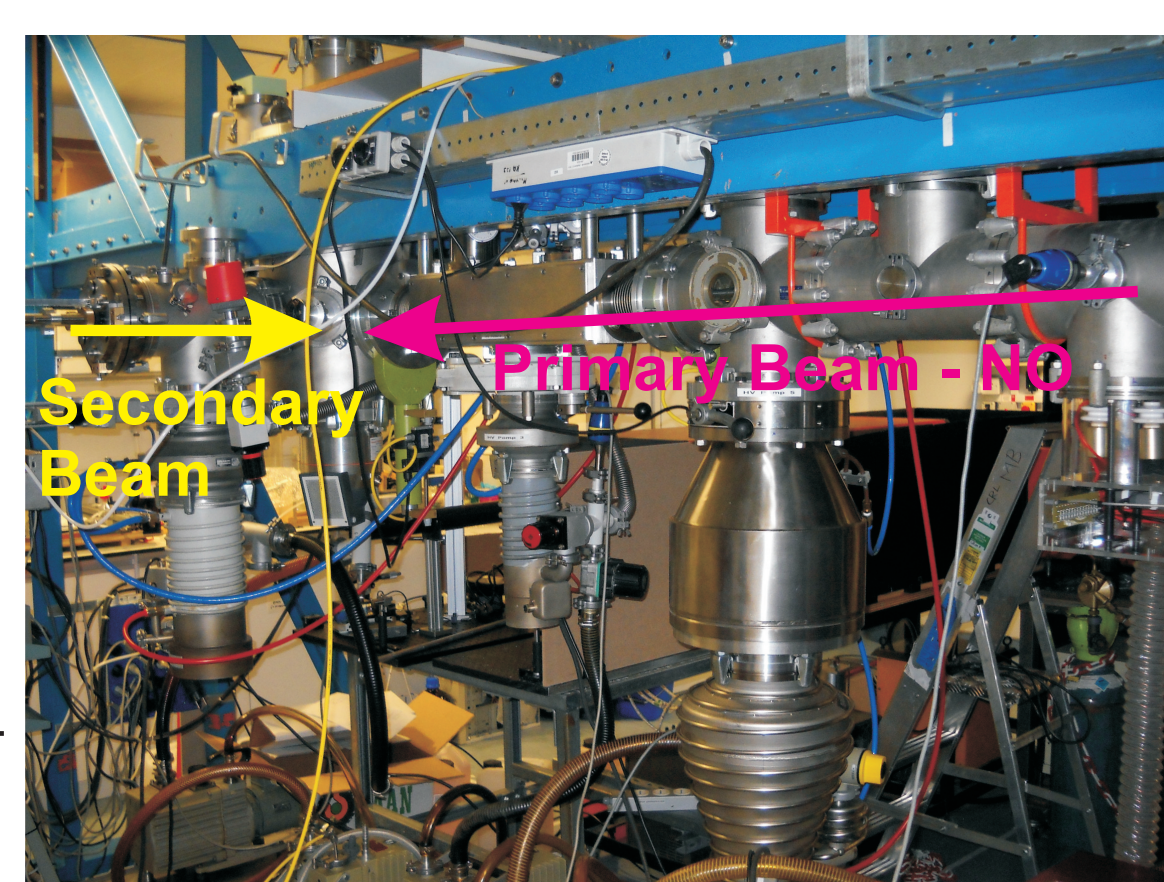


Ion images for scattering of NO with Kr. The intensity reflects the state-to-state differential cross section for the collision.

- 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 Krypton.
- The scattered NO molecules are then state-selectively excited and 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 theoretical quantum mechanical scattering calculations.

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

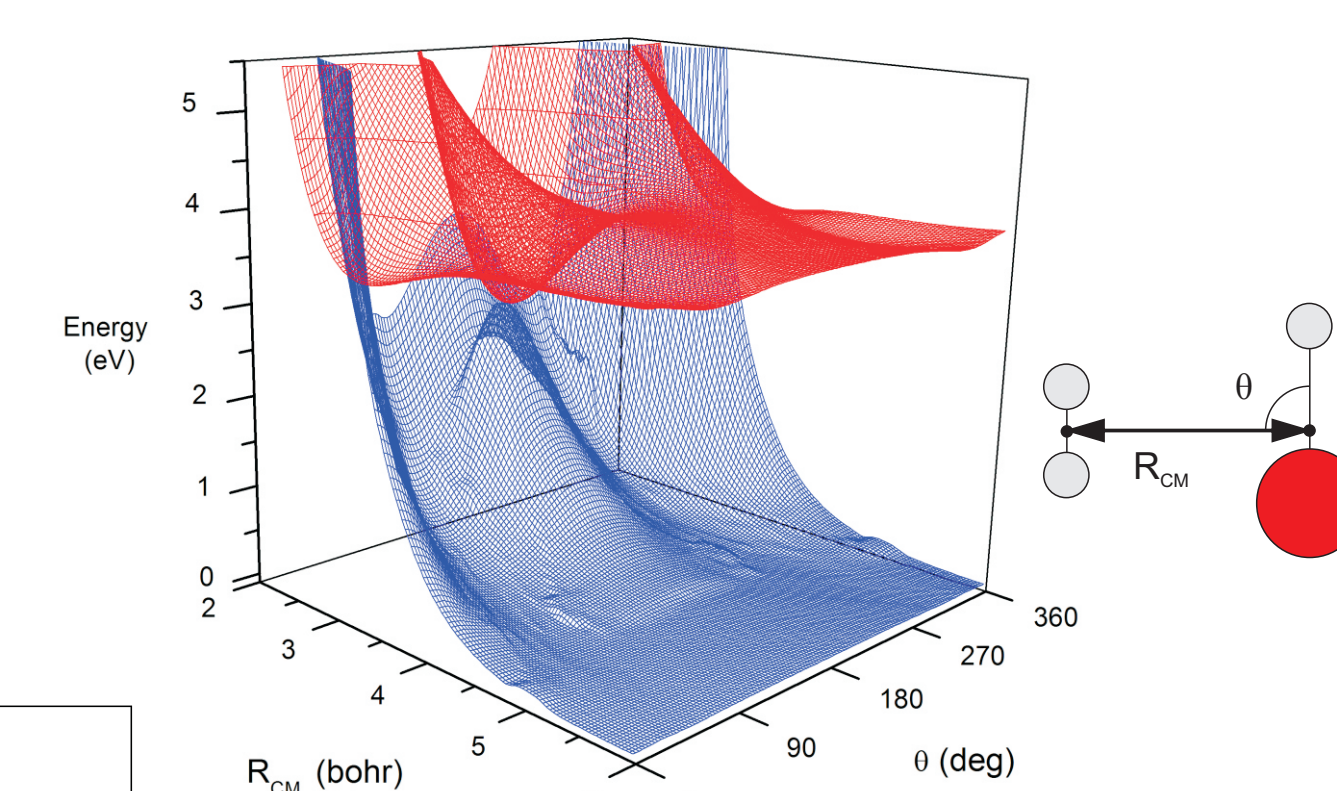
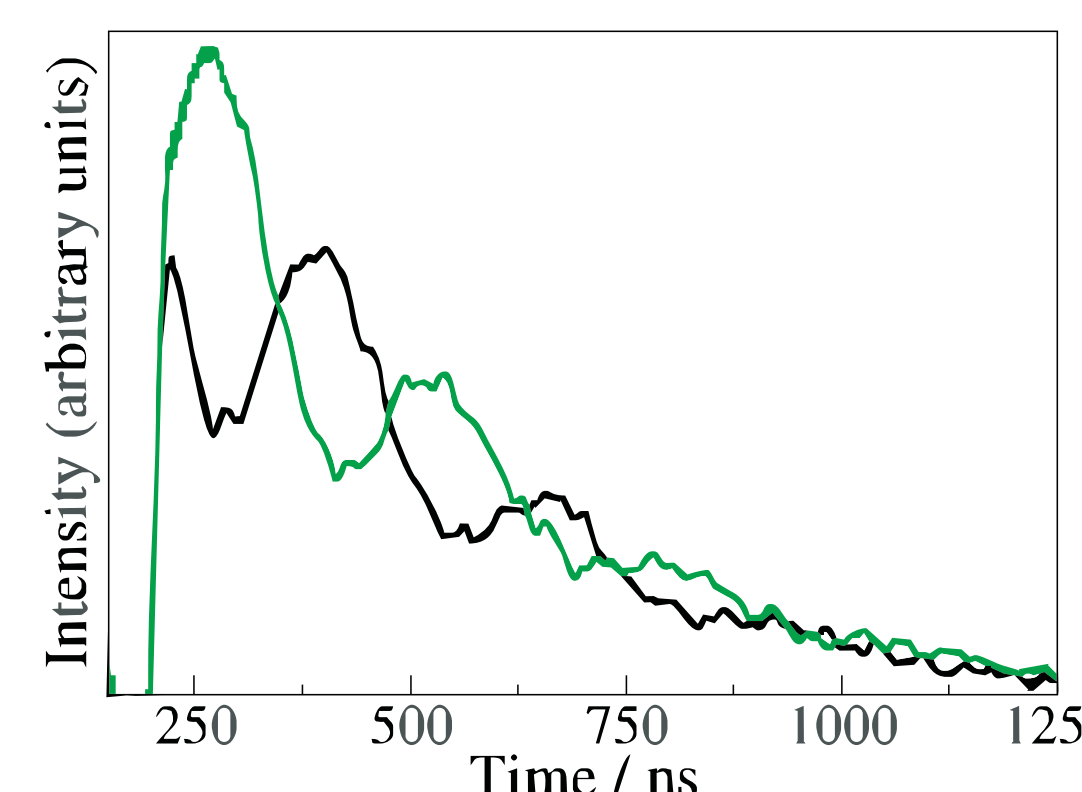


## Angular Momentum Polarisation

• Studying the effect of collisions on the angular momentum of molecules gives a sensitive insight into the dynamics of the process.

• By taking an initially polarised sample of OH(A) and colliding it with H<sub>2</sub> the decrease in the degree of polarisation can be measured.

• A weak magnetic field is applied which causes the angular momentum distribution to precess about the field axis resulting in modulations in the fluorescence intensity.

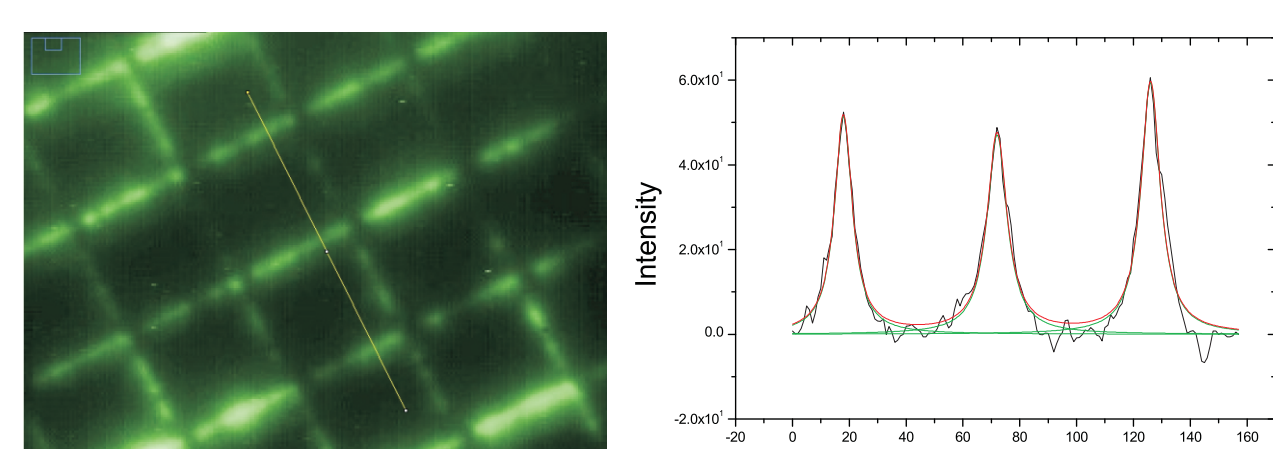


• The potential energy surface (PES) for this process (above) can be used to simulate the collisions.

• Trajectory simulations have been performed using newly developed 4-atom code.

## Imaging Mass Spectrometry

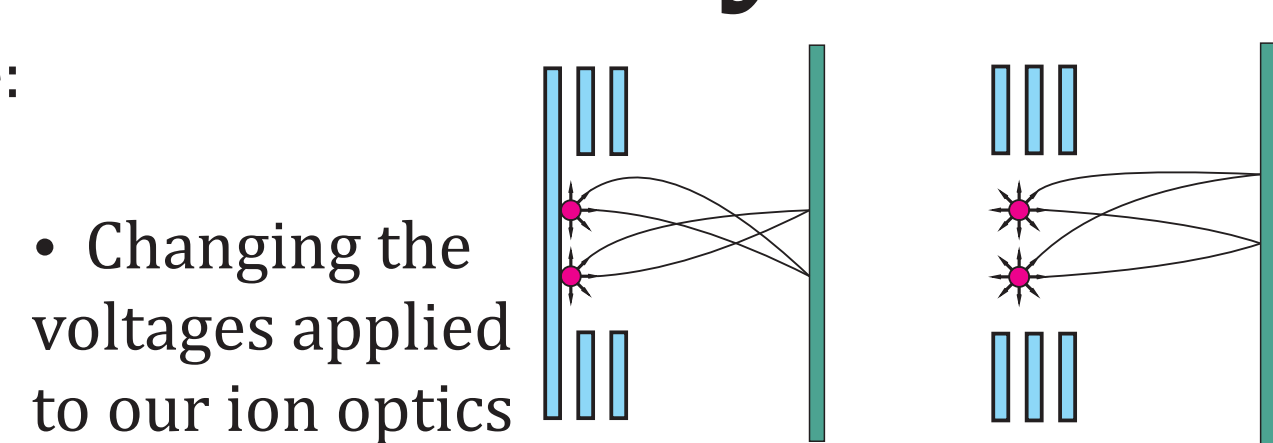
A chemical microscope:



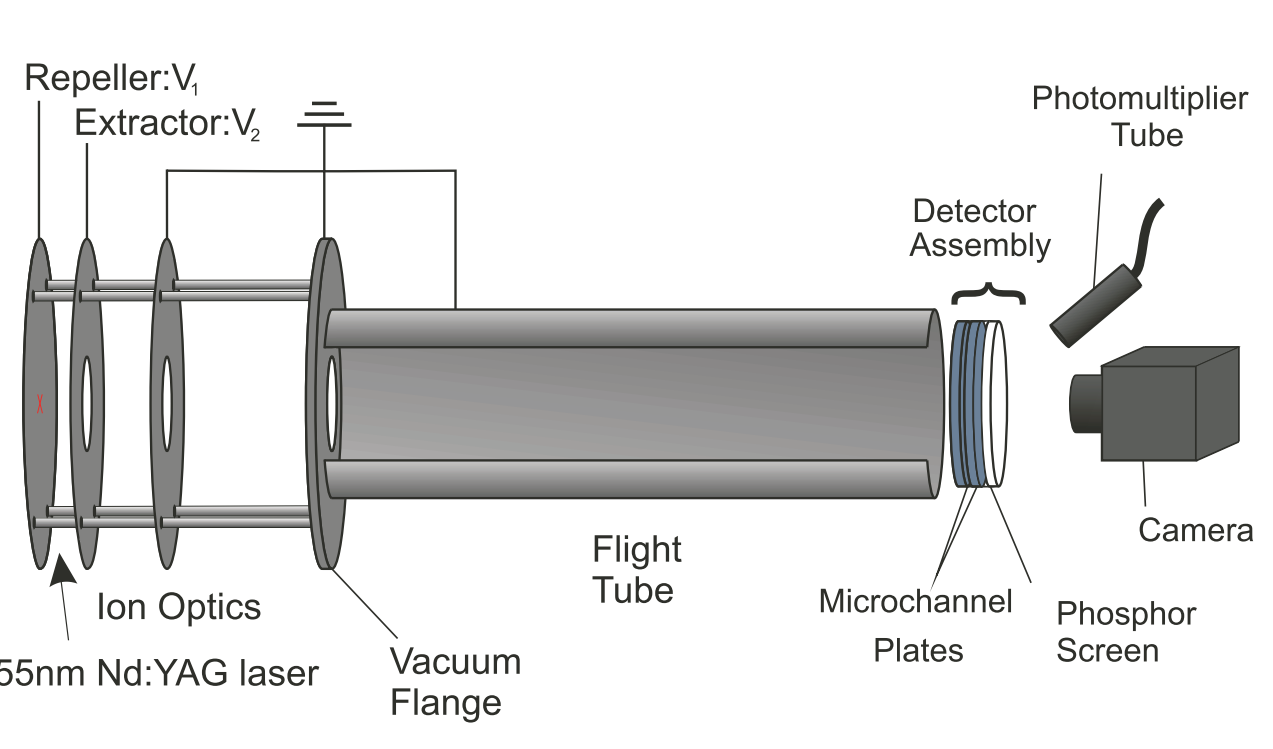
An ion image of a MALDI matrix sprayed into a grid pattern

• By desorbing and accelerating a sample we can conserve spatial information as well as time-of-flight (mass) information and create a chemical map of a surface.

• The spatial information can be used either to determine the position of proteins on a tissue sample, or to distinguish between multiple mass spectrometry experiments run in parallel.



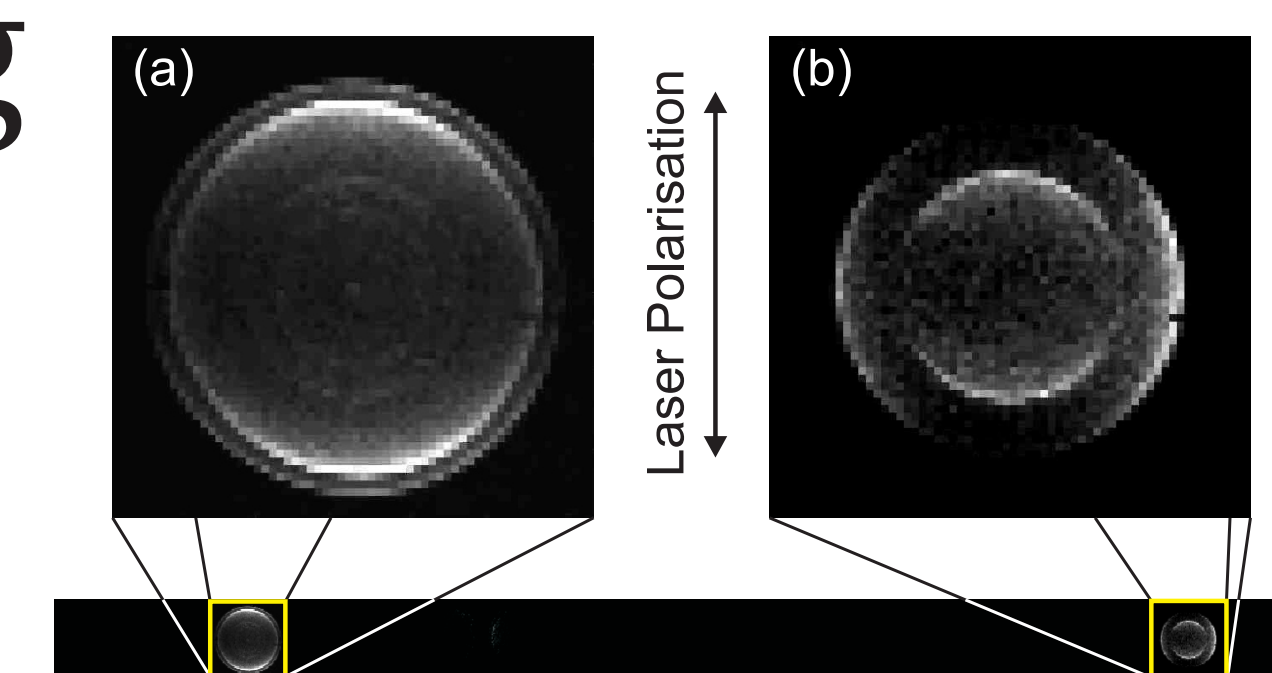
• Changing the voltages applied to our ion optics allows us to determine whether particles will be imaged conserving their spatial or velocity information.



## Coincidence Imaging

• Imaging multiple fragments from a single chemical event in coincidence can reveal detailed information pertaining to the underlying dynamics.

• We have developed a novel method of imaging both electrons and ions simultaneously in each experimental cycle using fast switching extraction potentials.



Simultaneously imaged electrons (a) and ions (b) captured using a Dalsa fast framing device.

## PImMS

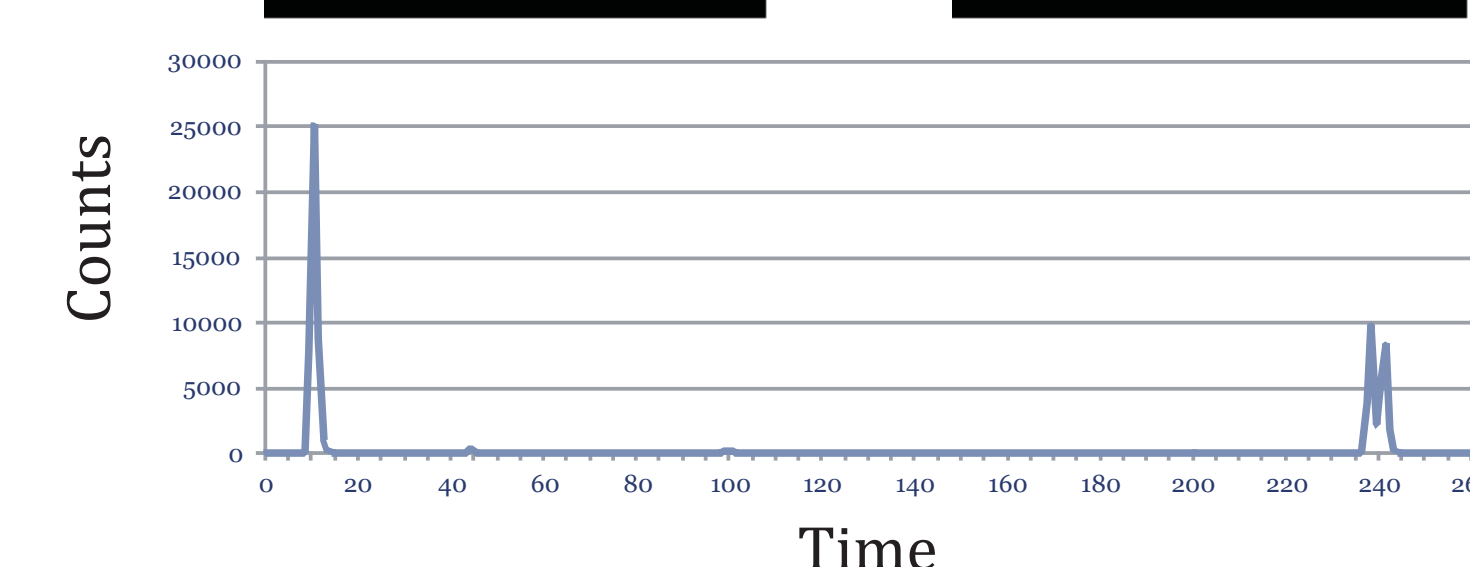
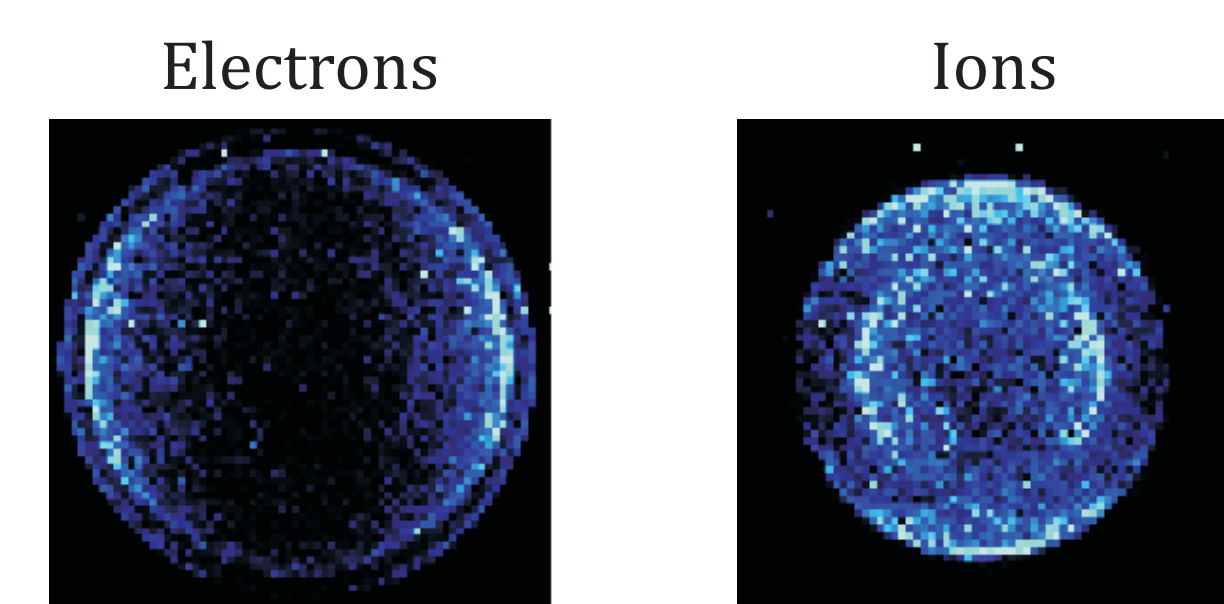
(Pixel Imaging Mass Spectrometry)

• The PImMS camera utilises novel CMOS (complementary metal oxide semi-conductor) technology to capture multiple images in a single experimental cycle.



The PImMS camera

• This allows for species of different masses to be imaged simultaneously in an ion imaging experiment.



For further information contact [mark.brouard@chem.ox.ac.uk](mailto: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!

