The Brouard Group

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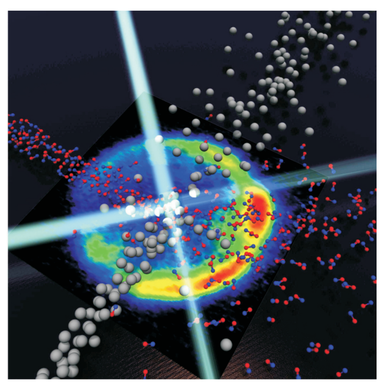
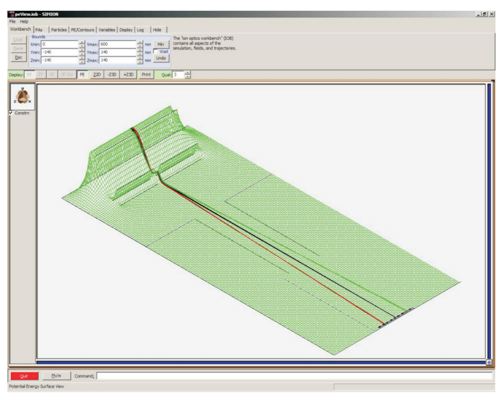
What we do

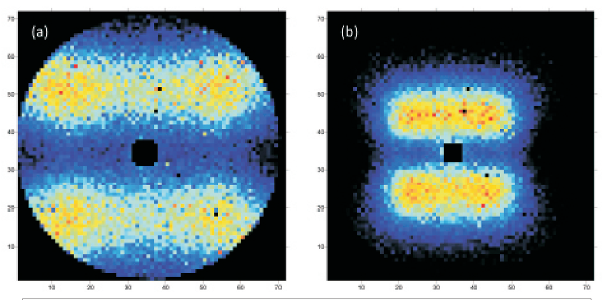
- Investigations into the dynamics of gas phase chemical processes and collisions using techniques such as ion imaging;



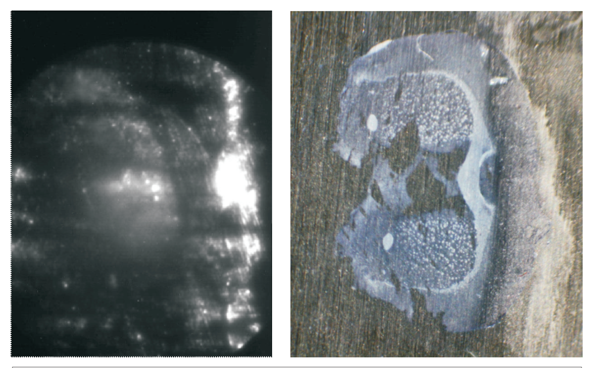


- Simulations and the development of models used to describe these fundamental processes;

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

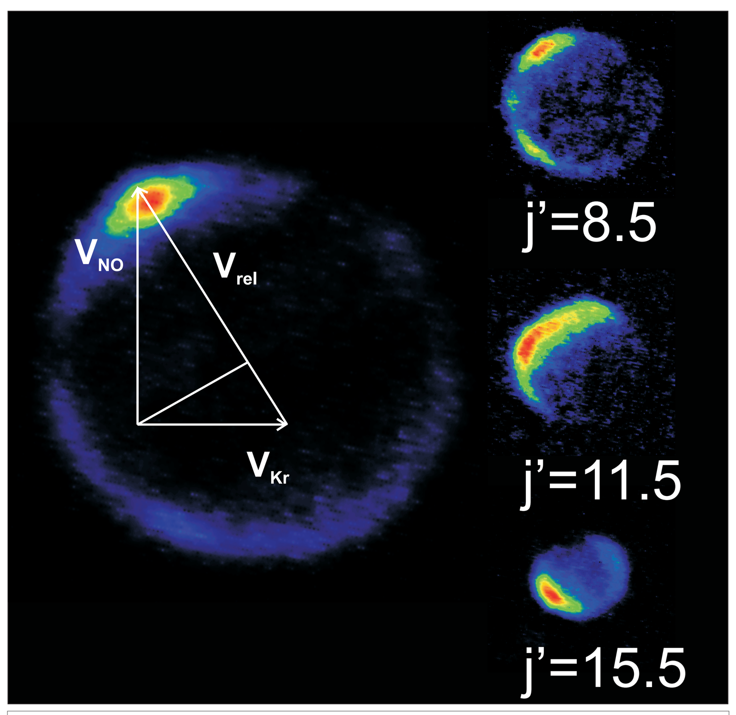


Raw ion images of the Br^+ and F^+ ion fragments following the Coulomb explosion of the DBrDFCyBPh molecule.



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

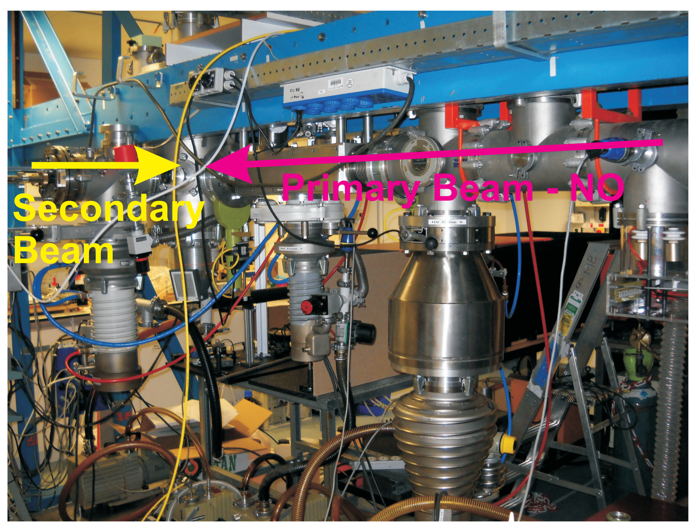
Quantum state-resolved scattering



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

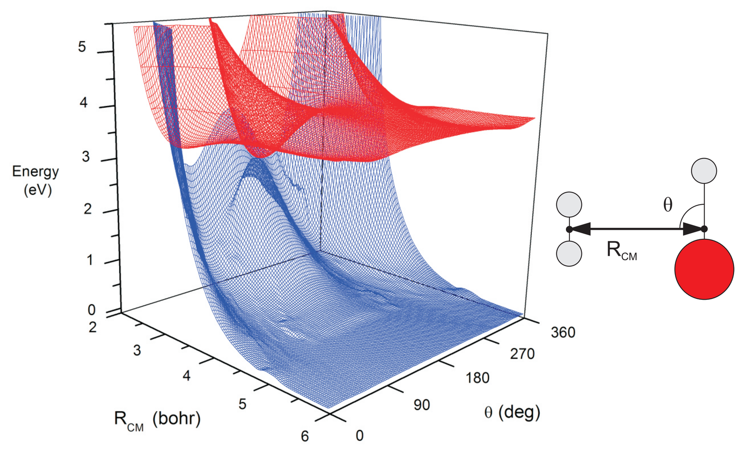
- The Blue Monster allows for observation of the angular distribution of fully quantum state-selected scattered molecules.
- A hexapole electric field selects the initial quantum state of the NO molecules in the primary beam.
- The beam of NO molecules is then intersected by the secondary beam containing krypton.
- The scattered NO molecules are state-selectively excited, ionised and accelerated onto a detector to give the images shown here.

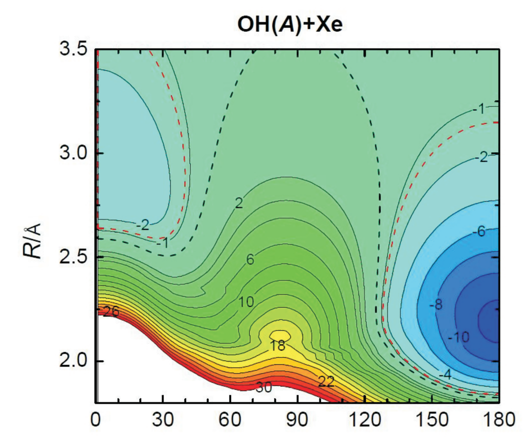
- For simple systems, such as NO + rare gas, the experimental differential cross sections can be compared with theoretical quantum mechanical scattering calculations.
- We plan to study more complex systems such as NO + diatomics by changing the gas in the secondary beam.

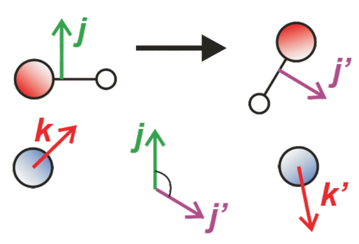


QCT Calculations

- QCT calculations are used to simulate the collisions studied experimentally by running trajectories over calculated potential energy surfaces.
- Over the course of a trajectory, the system is modelled both classically and quantum-mechanically.



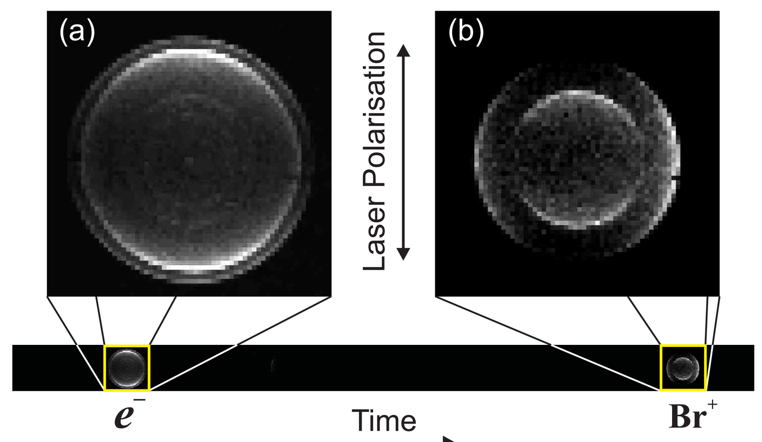




- The results of the QCT calculations are then compared with experimental data to assess the appropriateness of the QCT method.
- The QCT code has recently been expanded to incorporate non-adiabatic transitions between two or more potential energy surfaces. This is an important feature of OH + rare gas dynamics.

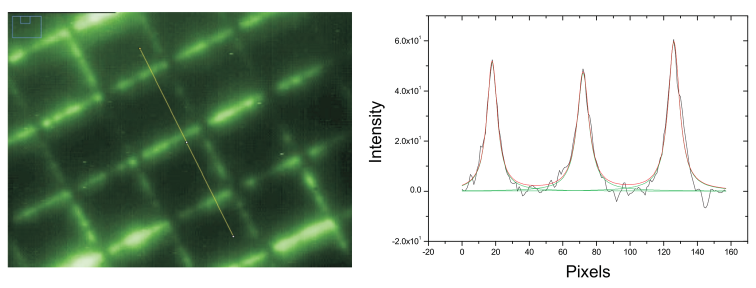
Coincidence Imaging

- Imaging multiple fragments from a single chemical event in coincidence can reveal detailed information about the underlying dynamics.
- We have developed a novel method of imaging both electrons and ions simultaneously in a single experimental cycle by using fast-switching extraction potentials.
- Recent experiments include studying the Coulomb explosion dynamics of molecules such as CS_2 and NO_2



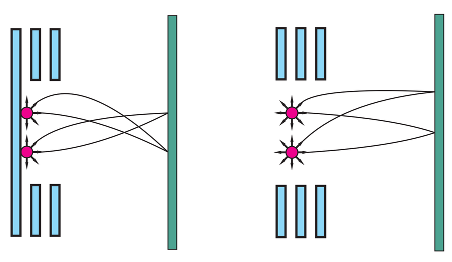
Simultaneously imaged electrons (a) and ions (b) captured using a Dalsa fast framing device.

Imaging Mass Spectrometry

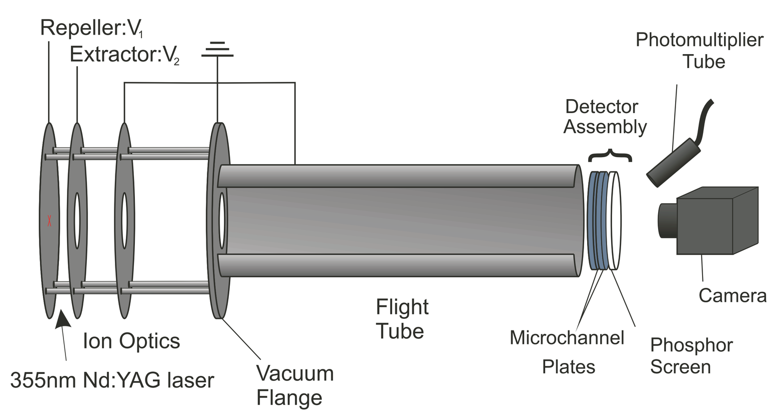


An ion image of a MALDI matrix sprayed into a grid pattern and the corresponding line profile.

- Changing the voltages applied to the ion optics allows us to determine how the particles will be imaged. Imaging can conserve either the spatial or velocity information of the ions.



- 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

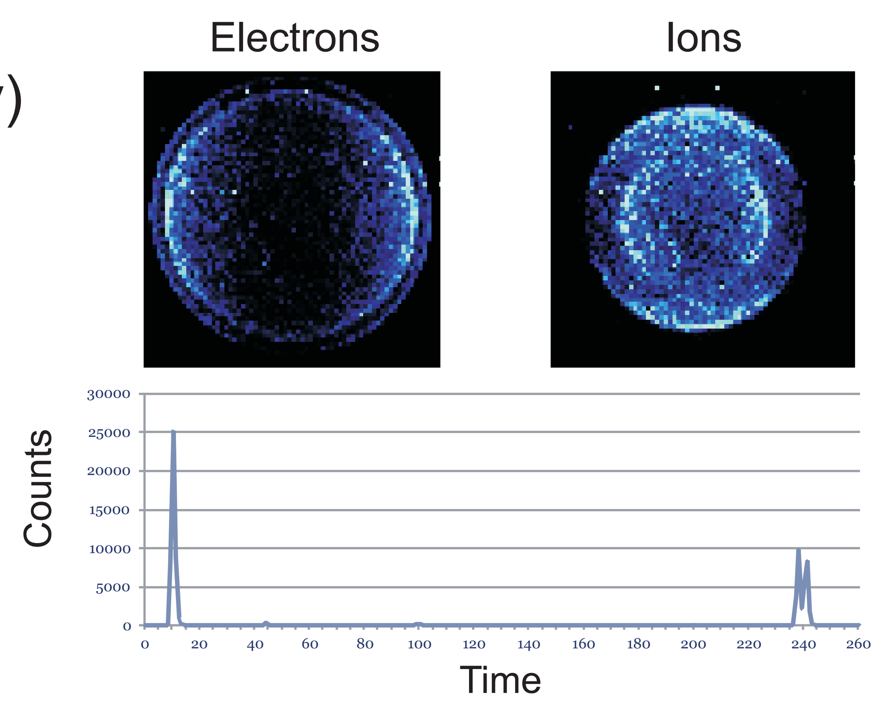


PImMS

(**P**ixel **Im**aging **M**ass **S**pectrometry)

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

- This allows for species of different masses to be imaged simultaneously in a single ion-imaging experiment.



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!