Quantum Conversations : Micro-Motion

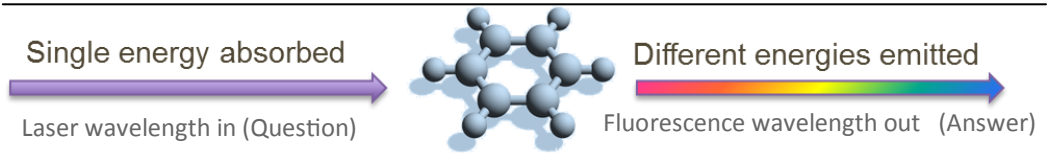
Patterns in Nature ~ Movement of molecules

An exhibition exploring the movement of molecules through the patterns they make using laser light in the Laser Spectroscopy and Molecular Dynamics Laboratory in the School of Chemistry and Physical Sciences, Flinders University.

Images from experiments using the world-class instrument built at Flinders University and the custom-made calculation software are compared with each other to find out about a molecule's changing shape as it moves.

The images from the lab are maps of energies within a molecule that can be 'seen' by recording the light emitted from molecules. They tell us about the energy it takes for a molecule to vibrate and rotate.

The images can be thought of as a "conversation" with a molecule. The molecule is asked a "question" by exposing it to laser light of a known energy. The molecule may take this light and "answers" by emitting its own light, but at differing energies. By recording the answers (emitted energies) to different questions (different probe energies) a map of the conversation is built up.



Dots and bands in the images are a direct consequence of Quantum Physics rules that apply to molecules and atoms (energy can only be released or absorbed in units called quanta).

Often the shapes of the energy patterns from the molecules studied appear to be like small moving creatures (butterflies, microscopic water life or sea life) or similar to energetic natural phenomena like waves, fireworks, sparks or swarming insects. This exhibition uses the images in ways to highlight the theme of movement to show how we can think about molecules around us as moving (tumbling, dancing) and being alive with energy.

The laboratory is a training ground for future researchers, and regularly trains students in experimental science. Where an image has been recorded by a student we have credited them with the work.

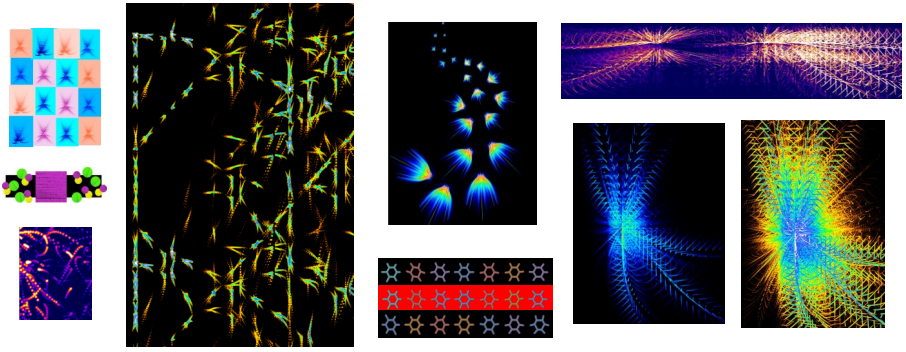
We hope you enjoy the images on display, and urge you to look closely at the images to discover underlying patterns for yourself.

Dr Ula Alexander | Dr Jason Gascooke | Prof. Warren Lawrance

(Laser Spectroscopy and Molecular Dynamics Team members, Flinders University)

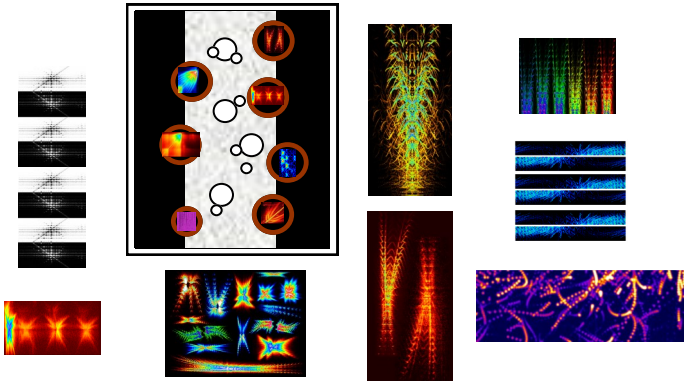
‘Quantum Conversations: Micro-Motion’ picture numbering guide

Left side of exhibition



1 2 3 4 5 6 7 8 9

Right side of exhibition



10 11 12 13 14 15 16 17 18

1. Toluene-Star Jumps

Arrangement of calculated possible toluene rotor images at 7K (-266°C)

This image is an arrangement of energy patterns calculated for the motion of toluene to see which image matches that from experiment. Each image is from a video made for the Australian Institute of Physics 'Art of Physics' National Congress 2014. The dots or banding in the 'star' images show the allowed energy of light absorbed/emitted from the toluene molecule as described by quantum physics. The arrangement represents the inspection process used in matching experimental data to the calculated data which is an important process. The tiles deliberately do not all align perfectly as a reminder that it is the process of looking for differences or misalignment when we are matching calculated data to experimental data.

2. Nitric Oxide – Argon Story

Experimental observation of nitric oxide at 7K (-266°C)
Recorded: July 27, 2012 ~ Student Experimenter: Abdullah Alsubaie

The image tells a story of the dynamic process of clusters containing nitric oxide and argon breaking apart. The gas temperature is so low that nitric oxide and argon can cling together. If the temperature was higher they would fall apart. The line patterns from experimental observations (in the centre rectangle and coloured circles) tell of free nitric oxide forming after it breaks away from being bound to an argon atom. These lines are superimposed on a "starry" background of dots due to nitric oxide molecules that were not bound to argon.

The breaking up of the nitric oxide-argon clusters is also told by moving from the left to the right of this piece. The purple and yellow circles (nitric oxide molecules) are linked to the green circles (argon atoms) in clusters that exist at low temperature but after receiving energy from a laser the cluster can now break apart and the argon (green circles) are now no longer linked to the nitric oxide molecules (purple and yellow circles). The free nitric oxide now tumbles at different speeds as shown by the lines in the experimental data. Each line corresponds to a different tumbling speed.

3. Fluorotoluene-Swarm

Detail from a calculated toluene 2DLIF image at 20K (-253°C) showing energy level changes for the propeller motion within para-fluorotoluene

A close-up view of the calculated energy pattern for para-fluorotoluene motion reveals a seemingly chaotic pattern. There is a balance of chaos and harmony reminiscent of fast moving insects or sparks from a firework leaving a trail of light. Each dot corresponds to an allowed energy change in the molecule, with the negative space corresponding to a forbidden energy. If our field of view were to zoom out then this apparent chaos within the overall para-fluorotoluene image would reveal a more ordered structure such as that seen in 'Fluorotoluene - Connect' of which this image is a small detailed section.

4. Fluorotoluene - Bird Walk

Overview of calculated para-fluorotoluene propellor motions image at 20 K (-253°C)

This image gives a much larger overview of the absorbed and released energies in para-fluorotoluene compared to other images in the exhibition. It shows the complexity of the vibration and twisting motion in the molecule. The dynamic activity of the para-fluorotoluene molecule produces an image that suggests the criss-crossing paths of busy animals such a birds who leave behind a trail of footprints. Just as the footprints are a map of activity of birds, this image is a map of the activity in the molecule.

Each of the bird-like footprint features in this image can be expanded and explored further. This expanded view is shown in the images "Fluorotoluene - Star Blue and "Fluorotoluene - Star Bright" so within patterns we can find more patterns. The fact that there is deeper structure within each of the "footprint" features is hinted at by the fact that these features are made up of many small cross-like shapes. These structures determined by quantum physics rules.

5. Fluorobenzene - Cool

Arrangement of calculated images of fluorobenzene from 298 K (25 °C) to 7K (-266°C)

This image was inspired by our journal cover article on molecular dynamics studies using 2D-LIF (2-dimensional laser-induced fluorescence). It aims to convey the feeling of the tumbling of fluorobenzene molecules as they expand into the vacuum chamber. It uses the calculated fluorobenzene energy pattern to show how the pattern is condensed as the molecules are cooled from room temperature to near absolute zero. The experimental apparatus cools the sample gas down to very low temperatures so that by the time the sample molecules intersect with the laser, they have reduced their rotational and vibrational energy significantly.

This image was included in Interalia Magazine Interalia Magazine's May 2016 "Micro-choreography" issue after a "call to artists and scientists for images of their work that aesthetically represent the dynamics of microscopic & molecular processes"

6. Benzene - Dance Mode

Models of the benzene molecule as it stretches, contracts and 'dances'.

The 'dancing' of the benzene molecule is by showing snapshots of 21 out of the 30 different ways that a benzene molecule can bend and stretch. Benzene is flat hexagonal ring of 6 carbon atoms each with one hydrogen atom attached. These atoms can move together in 21 different ways within the plane of the picture. The other 9 movements involve the molecule bending out of the plane of the picture and were not included. Each movement distorts the shape of the molecule and changes its symmetry. Of the 21 different movements in the plane of the picture, there are 4 different kinds of symmetries. Vibrations of different symmetries produce very different experimental images and we can use this to deduce what vibration we are seeing.

7. Fluorotoluene - Connect

Adjacent calculated para-fluorotoluene rotor features at 20 K (-253°C)

This image is of two neighbouring energy patterns in para-fluorotoluene which appear to be reaching out and connecting with each other. Through our work we have shown that the propeller motion and the vibration motion of the main ring with the molecule interact or 'talk' to each other very strongly. That is, they connect with each other. The extent to which this happens in molecules has not been realised until this work.

8.Fluorotoluene - Star Blue

Calculated para-fluorotoluene rotor motion at 20 K (-253°C)

This image shows one of the patterns made by the energy changes in the molecule para-fluorotoluene as the methyl group twists against the central ring structure while the ring vibrates. Each dot corresponds to photons released or absorbed by the molecule. The detail is determined by rules of quantum physics.

This image was included in Interalia Magazine Interalia Magazine's May 2016 "Micro-choreography" issue after a "call to artists and scientists for images of their work that aesthetically represent the dynamics of microscopic & molecular processes"

9. Fluorotoluene - Star Bright

Calculated para-fluorotoluene rotor motion at 20 K (-253°C)

This image reveals further detailed patterns below those seen in the same feature shown in 'Fluorotoluene –Star Blue'. This gives a sense of an energy burst with the all of the busy, complex patterns being displayed. Adjusting viewing levels and false colouring is an important part of analysing the data. Often the images are displayed in different ways to see both the very intense and weak features in order to get a complete understanding of the system.

10. Nitric Oxide –Tumble

Arrangement of experimentally observed nitric oxide image at 10K (-263°C).
Recorded: July 27 2012 ~ Student Experimenter: Abdullah Alsubaie

Nitric oxide (NO) data forms the basis of this image which is designed to mimic the motion of the molecule as it rotates or tumbles end-over-end inside the vacuum chamber. Each dot is represents observations of the photons of particular energies coming from NO molecules tumbling at different speeds. It uses alternating colour and a naturally occurring zig-zag pattern from the observed NO fluorescence data to create a tumbling effect. Due to the simple molecular structure of nitric oxide, it has a simple molecular motion and so creates a less complex fluorescence pattern compared to larger molecules.

11. Toluene – Three Amigos

Experimental observation of toluene rotor modes at 7 K (-266 °C)
Recorded: June 30, 2014 ~ Student Experimenter: Edwina Virgo

Experimentally collected images such as this from toluene often show shapes like butterflies in the fluorescence patterns. Cooling molecules reduces their congested patterns and allows the different features to be revealed. Weaker 'butterflies' behind the stronger ones are due to naturally occurring isotope carbon-13 replacing one carbon-12 atom in the toluene molecule. This subtle change in atomic mass changes the vibrational motion slightly and is seen as a weaker pattern shifted in energy compared to the brighter all-carbon-12 "butterflies".

12. Lab Space

Collage of copper, high-grade fused silica, aluminium and experimentally obtained 2DLIF fluorescence images from nitric oxide, toluene, fluorobenzene and benzene molecules.

'Lab Space' aims to remind us that images in the exhibition are fundamentally linked to experiments conducted by people in the lab. In experiments, the molecules being studied are in a vacuum chamber (symbolised by the silver metal) which has an environment inside like outer space hence the title, 'Lab Space'. Copper seals can be used to hold the vacuum inside the chamber. In the collage, used copper seals from the lab surround the light patterns collected from the molecules as they float in the dark void of the vacuum. The darkness inside the chamber is represented by the black components of the piece. This darkness is important for the extremely sensitive detector to be able to count only the individual photons coming from the molecules.

The 2DLIF (two-dimensional laser induced fluorescence) images within the copper rings were obtained using the lab apparatus to study (clockwise bottom left) nitric oxide, toluene, fluorobenzene, toluene, toluene, fluorobenzene and benzene molecules.

The white discs are high-purity (99.9999%), laser-grade fused silica (SiO_2) that can be polished into windows or lenses for use in experiments. They represent the clustering of the molecules in the cold gas cloud entering the vacuum chamber. For example, the larger discs represent disc-shaped benzene molecules and the smaller discs represent argon gas atoms. As the mixture of benzene molecules and argon atoms enters the vacuum chamber, the energy available for molecules to rotate and vibrate is reduced as they cool. The cooling is so much that the molecules and atoms can cling together without flying apart and form clusters. These clusters let us study weak bonds. These weak bonds have powerful effects since they are the first step in chemical reactions and help determine shapes of folding proteins so they are important interactions to understand.

13 Toluene- Mini-life

Calculated images of toluene rotor motions at 7K (-266°C).

The different motions of the spinning group attached to the central of the toluene molecule produce differently shaped features that are similar to butterflies, microscopic water life or insects. Theses familiar shapes of living creatures becomes ways of recognising the different energy patterns in analysing the spectra. A range differently shaped energy features are collected and arranged in the manner that insect samples would be collected and arranged for further study.

14. Fluorotoluene –Totem

Arrangement of detail from a calculated p-fluorotoluene rotor image at 20 K (-253°C).

This image is an arrangement of a close-up view of the allowed energy level changes associated with methyl rotor motion in *para*-fluorotoluene. The image is made from a section of the *para*-fluorotoluene energy pattern reflected about a central mirror plane. The centre of the image resembles a totem pole with radiating patterns of energy change emphasising the flowing nature of the patterns.

15. Toluene - Dancing Rotors

Arrangement of calculated (left) and experimental (right) toluene rotor at 7K (-266°C) recorded at 7K.
Recorded: June 24 2014 ~ Student Experimenter: Edwina Virgo

Images of fluorescence from the methyl rotor motion in toluene are combined to remind us of the link between theory and experiment. The left-hand side calculated and the right-hand side experimental images are rotated with respect to each other, as if they are twirling in a dance together. Does experiment drive theory, or theory drive experiment? When the two images are overlayed in the same orientation, the features in each image coincide showing that our model of the molecule's shape is performing well. Experiment is an important test of theory.

Toluene is a complex molecule to model spectroscopically because it has a methyl (CH_3) group attached to the central ring which can move by spinning or flexing against the ring. This image captures change in the torsional motion of this rotor group and the arrangement also suggests the spinning motion of the rotor.

16. Toluene – Fireworks

Arrangement of detail from a calculated image for a twisting motion with toluene at 20K (-253°C).

The different twisting motions in toluene create different energy patterns. The particular motion in this image creates a pattern with long plumes like a shower of sparks or fireworks. The image has been coloured and repeated like a row of colourful fireworks which also emulates the energetic motion of the molecule. Colouring of images is a useful way for inspecting and analysing the data to compare and contrast different features.

17. Fluorotoluene – Waves

Arrangement of detail from a calculated image for para-fluorotoluene rotor motion at 20K (-253°C).

The energy patterns obtained from calculation can be so detailed that they need to be looked at in sections. When viewing limited sections, the patterns can suggest familiar forms like waves in this case. A section of detail from the two patterns for the twisting motions in fluorotoluene used in 'Fluorotoluene - Connect' appeared to be like two waves crashing into each other. This image made from an arrangement of the 'crashing' waves is meant to convey also the dynamic energy of the molecule through more familiar energetic phenomena like ocean waves.

18. Fluorotoluene - Swarm (Large)

Detail from a calculated toluene 2DLIF image at 20K (-253°C) showing energy level changes for propellor motion within para-fluorotoluene.

This image shows a larger section of the para-fluortoluene energy pattern shown in "Fluorotoluene-Swarm" to show more of the trailing dot patterns that seem to map out the paths of flying insects such as fireflies. Each dot corresponds to an allowed energy change in the molecule, with the negative space corresponding to a forbidden energy.

Molecules in Motion

What is a Molecule?

Molecules are atoms bound together. The atoms in the molecule have a 3-dimensional arrangement that is determined by the laws of physics.

Tumbling, Spinning, Rotating

Isolated molecules are free to rotate in 3-Dimensions.

What Keeps a Molecule Together?

Electrons are the glue of a molecule. They are shared between atoms to "bond" them together.

Springy Bonds

Atoms in a molecule jiggle about. The bonds between atoms act as springs. The atoms vibrate.

Quantum Physics

Rules for the Tiny

The laws of physics for *small* things are different to those we experience in our *big* everyday world.

Quantisation

Quantum Physics often restricts a physical property (such as vibrations or rotations) to certain values—not all values are possible! The values are *Quantised*.

Strange Effects

Quantum Physics reveals several strange concepts that are very different to everyday experience. However, these concepts are predicted mathematically and shown experimentally.

Rules for Changes

If a physical property is quantised, then there can be rules about what changes are possible. These are *Selection Rules*.

Quantised Molecules

Vibrations

Atoms within a molecule must vibrate in a choreographed fashioned as directed by Quantum Physics.

There are only a limited number of *vibrational motions*; this is governed by the number of atoms.

A molecule can only vibrate with specific amounts, or *quanta,* of a vibrational motion.

Vibrational energy is quantised.

When is zero not zero?

Atoms in a molecule can never stop moving. The lowest vibrational energy possible in the molecule still requires the molecule to vibrate—called *Zero Point Energy*.

Rotations

The entire molecule can rotate in space, but only in a way that satisfies the laws of Quantum Physics.

A molecule can only rotate with specific amounts, or *quanta,* of a rotational motion.

Rotational energy is quantised.

Excited Molecules

A molecule not rotating and at its lowest vibrational energy is said to be in its *Ground State*. Otherwise, it is called *Excited* or in an *Excited State*.

Interacting with Light

Particles of Light

Light is made up of small packets of energy called *photons*.

Each photon has a fixed energy. In the visible spectrum, red photons have low energy, whilst violet photons have high energy.

Absorption of a photon increases a molecule's energy.

Release of a photon (called *fluorescence*) lowers a molecule's energy.

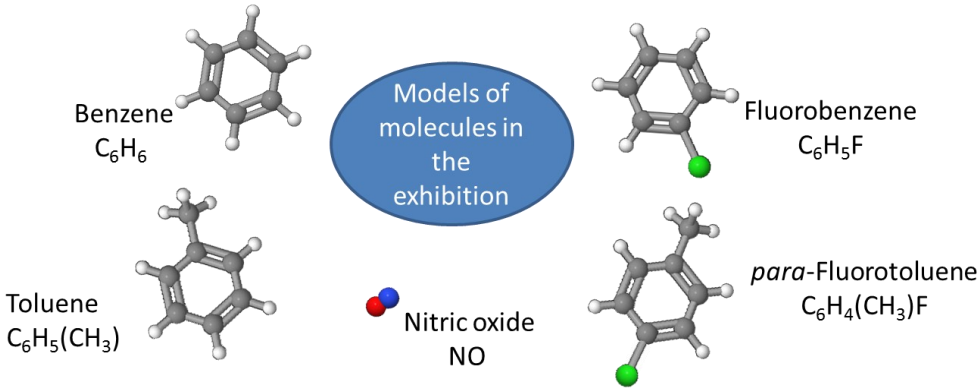
A Change of Motion

When molecules absorb or release light (a photon) they can change their rotational energy. They may also change to a different vibrational type and energy.

Quantisation of molecular motion means that only certain energy changes are allowed by the molecule.

Incoming and outgoing photon energies must match the energy gaps in the molecule.

By observing the energies of light that are absorbed, and measuring the energies of light that are emitted, an energy map is produced that is a "fingerprint" of the molecule's molecular motion.



Each molecule dances, jiggles and vibrates in its own way.

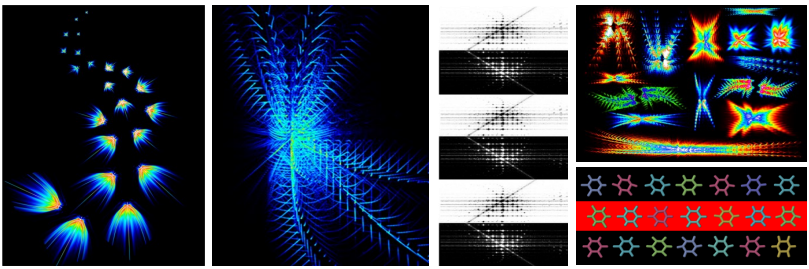
More atoms in a molecule means more there's more ways it can move. More ways to move means more complex energy patterns as seen in the exhibition.

- Nitric Oxide with 2 atoms vibrates in 1 way.
- Toluene with 15 atoms vibrates in 39 ways.

Toluene's structure has a benzene ring with a methyl (CH_3) rotor group that is like a propeller that can spin while the whole toluene molecule is spinning. This mixture of different motions makes it really complex to model.

Molecules like toluene are studied because they are prototypes for even more complex molecules such as those found in biological systems.

Quantum Conversations: Micro-Motion



July 27 - Sept 1 for SALA 2016

Dynamic motion of molecules explored through their quantum energy patterns as seen in the Laser Lab, Flinders University.

July 27 – Sept 1 SALA South Australian Living Artists Festival 2016

The Artisan Café (behind Bendigo Bank)
252 Main Rd, Blackwood | Ph (08) 8278 9888
www.TheArtisanCafe.com.au

Opening night Thurs August 11, 6-7.30pm.

Visit www.quantumconversations.net/projects/sala-2016

Presented by Dr Ula Alexander

SALA

national science week 2016