Femtochemistry and Femtobiology (ULTRA)

An ESF scientific programme

The European Science Foundation acts as a catalyst for the development of science by bringing together leading scientists and funding agencies to debate, plan and implement pan-European initiatives.

The desire to explore our surrounding world has always been one of the strongest characteristics of human nature. Columbus and the great explorers travelled outwards and discovered new continents in the 16th century and Bohr, Einstein, Rutherford, Curie and many others travelled inward to explore the secrets of the atomic world in the 20th century.

Explorers use ships, planes or spacecraft to travel outward and they use increasingly sophisticated scientific tools to travel inward into the world of atoms and molecules. Here at the beginning of the 3rd millennium we have microscopes allowing us to see single atoms and telescopes allowing us to see the edges of the universe. At the end of the 20th century a fascinating new tool, the femtosecond laser, was developed. The femtosecond laser provides us with ULTRA short light pulses, allowing the motion of atoms and molecules to be captured as if they were filmed. To have, not only the structure of atoms and molecules, but also their motion, is of unique importance in our quest to understand and control chemical and biological processes.

The ULTRA Programme, sponsored by the European Science Foundation, is a collaborative effort among the leading European laboratories engaged in using femtosecond laser pulses in chemistry and biology, a field of research with its own name: Femtochemistry and Femtobiology. In this brochure we give a brief introduction to the field and illustrate the activities within the Programme with a few illustrative case stories.

Aims and objectives

By focusing on the ultrafast timescale of femtoseconds (1fs=10^{-15}), this Programme's aim is to improve our understanding of dynamics – how systems move between apparently equilibrated structures, changing their chemical composition and performing biological functions on the way. It will exploit new and emerging extensions of ultrashort pulse applications such as time resolved (fs) single molecule spectroscopy, scanning two-photon fluorescence microscopy and fs X-ray pulse generation.

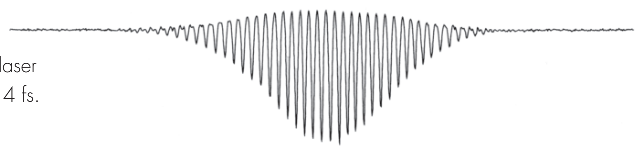
Introduction

The ultrafast time scale of femtoseconds is the time scale of elementary chemical reactions and of electronic and nuclear motions in molecules: when chemical bonds are formed or broken during chemical reactions, when molecules rearrange to form new molecules, or when energy is transported from one molecule to another, all these processes take place on a femtosecond time scale. Thus our fundamental understanding of chemical and biological processes ultimately relies upon a thorough understanding of the ultrafast processes.

Femtosecond lasers have been applied to most areas of chemistry and many molecular mechanisms in biological systems have been established. With the emergence of new and highly reliable techniques, completely new applications of ultrashort pulses come within reach: Time resolved single molecules spectroscopy, scanning two-photon fluorescence microscopy, X-ray pulse generation, non-thermal micro-machining and coherent control of reactions, etc. All these new extensions of ultrashort pulse applications will, together with existing applications, be important topics of this ESF Programme.

1 femtosecond (fs) corresponds to 0.000000000000001 second, in scientific notation 10^{-15} second.

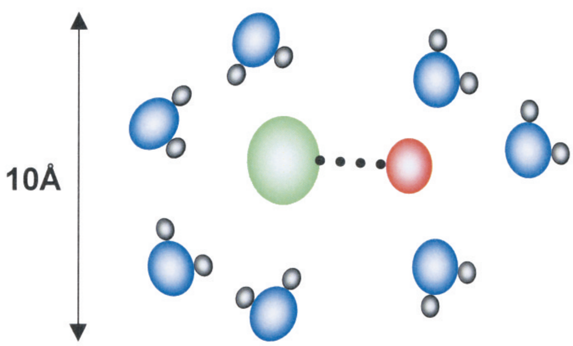
- In 1 fs light will travel only 0.3µm.
- 1 fs is to 1 sec. what 5 minutes is to the age of the universe
- The shortest laser pulse to date is 4 fs.



Femtosecond case stories

Taking pictures of chemical reactions

The art of high speed photography started in 1877 when Eadweard Muybridge, as a result of a bet, took a series of snapshots of a galloping horse, to prove that the horse at some point has all four hooves off the ground. By freezing the motion of the horse one can directly study the pictures and learn about gallop.



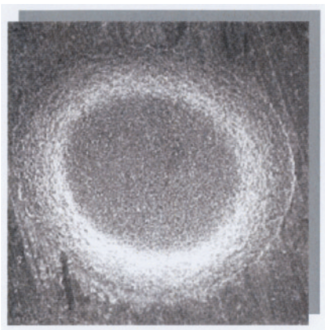
When the chemical bond between the red and green molecules above are broken the molecules move apart at a velocity close to 1 km/s. With the femtosecond laser we can directly monitor this motion and get detailed information on how and how often the molecules collide with neighbour molecules. In particular the communication between the molecules is of prime importance in order to get a deeper understanding of chemical reactions. In simple terms we have to learn the language spoken among molecules. In principle we know quite well the structure of individual molecules, but we only have a limited insight into way in which molecules interact with each. Femtosecond lasers have proven to be a very capable translator of the molecular language.

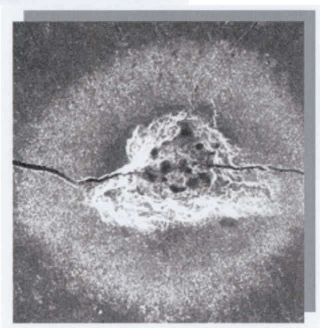
In a similar way it would be desirable to freeze the motion of atoms and molecules while they are involved in chemical reactions. One of the scientific milestones achieved using femtosecond lasers was the use of these lasers to take pictures of chemical reactions while they take place. The Nobel prize in chemistry 1999 was awarded to Ahmed Zewail for the pioneering use of femtosecond lasers to study chemical reaction.

Micromachining

fs-pulses can be very intense and therefore have unusual properties that are distinct from other lasers.

When conventional lasers are used to machine (cut, drill, etc.) materials, they work through absorption of the powerful laser light. When femtosecond lasers are used for machining, they can use much lower power since the laser light is concentrated in an ultrashort pulse. With femtosecond lasers it is possible to machine without heating the material at all. This has enormous implications for the use of lasers for surgical procedures, as it is possible, for example, to remove tissue without inflicting any damage to nearby tissue. Presently this is used for experimental surgery in the eyes and in the spinal cord.





The two pictures show the difference between micromachining a tooth with a standard laser and a femtosecond laser.

Alignment of molecules

In a chemical or bio-chemical reaction, the orientation of the reacting molecules plays a determining role for the outcome of the reaction. Using intense ultrashort laser pulses, a technique has been developed to control the alignment and orientation of molecules. A powerful, but non-resonant laser is used to orient the molecules. Using linearly polarized light, they align the molecular axis of the molecules, and by adding an elliptically polarized light beam, it is possible to control the orientation of the molecular plane in medium-sized organic molecules. The degree of alignment is monitored using ultrafast Coulomb-explosion of the molecules.

Ultrafast relaxation in water

One of the most important questions in chemistry and biology is how, and how fast, energy is transferred in, and in between molecules.

In a series of femtosecond experiments it has been investigated how intermolecular energy was transferred in liquid water. Using an infrared femtosecond pulse, the OH-vibration was excited in liquid water. The subsequent fate of the excited water molecule was followed using a delayed and polarized infrared probe pulse. This enabled the researchers not only to see how fast the water molecules rotate, but also how fast the energy is transferred from one water molecule to its neighbour. Surprisingly, this energy transfer time in liquid water is extremely short, less than 100 fs, indicating an extremely efficient mechanism for energy transport in liquid water. The mechanism is linked to the unusual structural properties of liquid water, dominated by a network of strong hydrogen bonds between the individual water molecules. Given the importance of aqueous environments, in particular in biology, the discovery of the ultrafast energy transport among OH-bonds also provides new insight into the possible energy transfer between, for example, proteins dissolved in water.

Ultrafast molecular biology

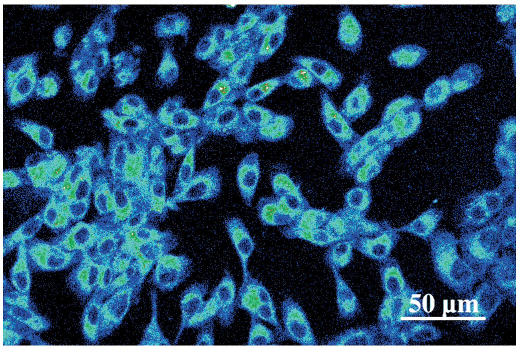
There is no doubt that molecular biology will play a dominating role in the 21st century. Many scientists predict that molecular biology will dominate the 21st century as physics dominated the 20th century. A key element in this development is the humane genome project where researchers all over the world work to determine the DNA structure of the human chromosomes.

Femtosecond lasers also play an important role in determining how bio-molecular structure and dynamics work together to define function. An interesting observation is that in most, if not all, biologically important processes, like photosynthesis, the uptake of oxygen in the blood, vision, etc, start out in an initial, very fast (femtosecond) step. The purpose of the first step is to secure that no other interfering processes can take place and the faster the step, the more likely is the desired outcome of the reaction.

A good example of this principle are the fast structural changes taking place in the molecules responsible for vision. Using femtosecond lasers, researchers have demonstrated how an ultrafast single twist around a chemical bond in the retinal molecule is responsible for initiating the complex bio-molecular response eventually giving rise to a vision stimuli in the brain. For the well-adapted eye (night vision) the sensitivity to individual light particles (photons) is extremely high, primarily because of the ultrafast initial twist. Chemists call this "twist" a cis-trans isomerization, which is shown below for the retinal molecule.

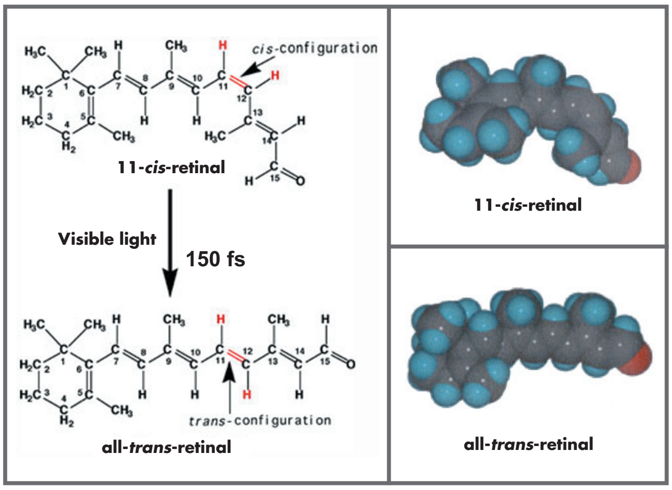
Non-Linear Microscopy

In the last few years femtosecond pulses have caused a minor revolution in the development of microscopes for bio-medical applications. Again, the fact that the light is concentrated in a very short time-interval makes femtosecond laser light distinctively different from light from normal sources.



The picture shows a cell culture which has been exposed to *photofrin*, a photo-activated drug used in the treatment of cancers. The image was obtained using a non-linear microscope and images like the above help researchers to gain more knowledge of the actual mechanism by which photoactivated drug works. © M Nichols, Developmental Resource for Biophysical Imaging Opto-Electronics, Cornell University

In non-linear microscopy, the femtosecond laser is used to excite bio-molecules and the light emitted from these molecules is used to form an image. The lasers operate at long wavelengths (>800 nm) which can penetrate into the tissue. For a normal laser operating at 800 nm there is not enough energy to excite the bio-molecules. However, with focussed ultrashort pulses it is possible to excite the bio-molecules via absorption of two photons.
With non-linear microscopy a good spatial resolution can be achieved in all three dimensions, enabling sectioning of the studied sample and generation of three-dimensional pictures.



Femtosecond lasers provide new insight into the relationship between structure and dynamics and function of large bio-molecules.
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ULTRA activities

The ULTRA Programme offers support for the organisation of **schools, practical courses** and **workshops** in the field of femtochemistry and femtobiology and issues an annual call for proposals for these activities. Potential organisers of schools, practical courses and workshops are strongly encouraged to choose **focussed themes**. Examples of subjects of great current interest within the scope of the ULTRA Programme are:

- Electronic energy transfer and charge separation
- Short pulse generation
- Ultrafast processes in organic and semiconducting materials
- Bioimaging
- Biological reaction dynamics
- Liquid dynamics
- Vibrational energy transfer
- Wavepacket dynamics and coherent control
- Elementary chemical reactions
- Coherence in chemistry and biology

The ULTRA Programme also offers support for **short-term visits** of one week to one month, to stimulate co-operation between research groups in different European countries. Priority will be given to younger researchers (eg PhD, post-docs) but applications from senior researchers will also be considered. These visits may also be used for learning new techniques.

Further information on activities supported by the ULTRA Programme and on how to apply for support is available at *www.esf.org/ULTRA*.

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For the latest information on this programme consult the *ULTRA* home page:
http://www.esf.org/ultra or *http://www.chemphys.lu.se/esf/index.htm*

Cover picture: Ice, water and clouds: water is essential to our existence and many new aspects of water have been revealed using femtosecond lasers.
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