PHYSICAL CHEMISTRY

When dreams come true...

Filming a chemical reaction live using bursts of X-rays

All chemists dream of being able to see molecules dance – to follow their transformation during a chemical reaction. For researchers at DTU Chemistry, the dream became a reality when they recently went to Japan to one of the world's first X-ray free-electron laser facilities. This could open the door to new and far more efficient and effective chemical processes.

It has only recently become possible to actually "film" what happens in a molecule when it changes structure. The new so-called X-ray free-electron laser facility, XFEL for short, can, with the help of X-rays, take pictures fast enough to capture the myriad processes that take place in a molecule after a chemical reaction is initiated. The molecular dynamics during the chemical reaction occurs on the femtosecond time scale, which is extremely fast. The ratio of a femtosecond to a second is the same as between a second and 32 million years! The Japanese X-ray laser system SACLA is only the second of its kind in the world – the first one opened at Stanford University in the USA two years ago. A third, located in Hamburg, will be ready in a few years.

Associate Professors Niels Engholm Henriksen and Klaus Braagaard Møller from the research group Theoretical, Computer and Femto-Chemistry at DTU Chemistry have been involved since the very start, when the research project was started at the Centre for Molecular Movies, a centre of excellence funded by the Danish National Research Foundation. Together with DTU Physics, they have, over the past few years, been building up a body of expertise in these large high-tech X-ray facilities.

"There are endless possibilities for the new large X-ray facilities if we can achieve even a modicum of the success that traditional X-rays have had in contributing to our understanding of the molecular structures of, for example, proteins," says Associate Professor Klaus B. Møller from DTU Chemistry.

"The ultra-short X-ray pulses make it possible for us to see still images of molecules in motion, thereby shedding light on fundamental processes in areas such as chemistry, biology and technology," he continues.

Femtochemistry

The background for Niels Engholm Henriksen's and Klaus B. Møller's research is femtosecond chemistry, which lies somewhere on the border between chemistry and physics. The research consists of the development of concepts and ideas based on the laws of quantum mechanics translated into equations and computer programs – in order to detect ("film") and control ("direct") atomic motion while chemical reactions are taking place. Detection and control of atomic motion is based on the interaction between molecules and ultra-short (femtosecond) flashes of electromagnetic radiation, which can both provide the required time resolution and, through the coherent excitation of intrinsic quantum states, create molecular states which cannot be created through conventional heating.

The Japanese Adventure

In the Japanese highlands there is a 700-metre-long tube through which compact bunches of electrons run at almost the speed of light. The electrons are exposed to undulator magnets so that they emit extremely short-lived X-ray pulses that are sent into the sample that the researchers have brought with them from Denmark.

PhD student Asmus Ougaard Dohn from DTU Chemistry got a unique chance to take part in research at the facility (SACLA) in Japan, where he and his supervisor Klaus B. Møller went recently, together with researchers from DTU Physics as well as from Sweden and Hungary. They had just 72 hours of so-called «beam time» to record how a single charge would move through the sample – in a specially designed molecule – after it had been illuminated by a laser pulse.

Time spent using an XFEL is expensive. Operating costs are high. At the facility at Stanford (LCLS), it costs approx. DKK 100,000 per hour to run an experiment – whereas the figures for SACLA in Japan are slightly lower.

«Having access to such a large and expensive facility gives us very good "value for money". We're incredibly lucky to be able to send our PhD student Asmus Ougaard Dohn there so he can use the data for his project back here at DTU,» says Niels Engholm Henriksen, who is co-supervisor on Asmus' project, which is co-funded by DTU Chemistry and the Lundbeck Foundation.

«We have a unique opportunity to gain valuable experience which will put us in a good position in relation to the upcoming facility in Hamburg,» he continues. A facility that researchers in Denmark are very much looking forward to being able to use. When completed the expected cost will be about 1 billion euros!

The future looks bright

There is, however, no guarantee that researchers will succeed in creating their own molecular movies at these facilities; and even if they do, they may not understand what they have filmed. But in Japan, Asmus Ougaard Dohn did actually manage to create useful data to bring back for his PhD project on ultrafast molecular dynamics. In the 63rd hour, researchers broke out into ecstatic dancing, as the computer screen showed a graph – amid the noise and mess – indicating unequivocally that this was a time-resolved scattering signal – evidence that they had captured "something moving in the molecule" that they could work on. The series of scattering patterns can be combined to form a kind of movie of how the molecule behaves as the electron moves from one end of the molecule to the other.

"Our overall goal is to develop a translation device between the data we record and images with atomic resolution in both time and space that can show molecules' structural dynamics during chemical reactions at the same moment they occur. If successful, it will give an unprecedented insight into the world of chemistry, and the results may lead to new ways to optimize chemical reactions," says Klaus B. Møller.

"Our research is driven by pure curiosity, combined with a clear perspective on practical applications," adds Niels Engholm Henriksen. But there is still a long way to go before using the new facilities can be considered a "routine job". Most of the work is currently going into developing the necessary computational technology to interpret the data produced; and DTU Chemistry has been there right from the start.

FEMTO11

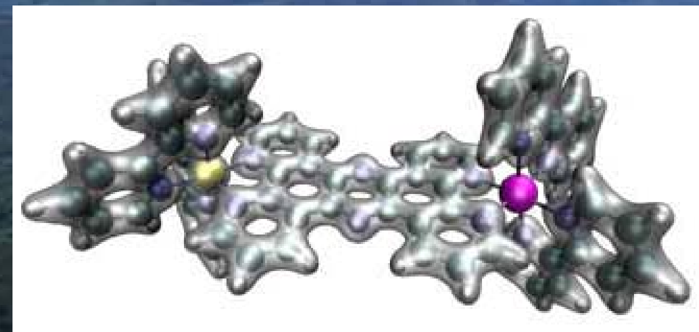
The Femtochemistry Conference

The 11th Edition of the International Femtochemistry Conference - Frontiers of ultrafast phenomena in Chemistry, Biology, and Physics - will take place in Denmark, from 7 to 12 July 2013. The scientific venue will be at DTU.

FEMTO11 will bring together 200-300 scientists from all over the world to present and discuss the most recent advances in femtosciences, including structural dynamics studied by XFEL facilities, reaction dynamics, coherent control, solvation phenomena, liquids and interfaces, fast processes in biological systems, strong field processes, attosecond electron dynamics, and aggregates, surfaces and solids with contributions from both theory and experiment.

Furthermore, the conference will open with a keynote lecture by Nobel Laureate Ahmed Zewail well known to both Associate Professors Niels Engholm Henriksen and Klaus B. Møller from DTU Chemistry who have collaborated with the Nobel Laureate for several projects during the years. "We are very proud and happy to host this prestigious Conference here at DTU, " says Conference Chairman Niels Engholm Henriksen from DTU Chemistry. "It's a unique chance to positioning our research in Denmark as an important player on the international scene of femtosciences."

We welcome you to participate, please learn more at the website: **www.femto11.com**



The measurements take place in the experimental hutch at the end of the 700 m long accelerator/undulator tube. Although XFELs are among the most advanced technical installations, a last minute protection of the equipment from air was made by a common waste bag and duct tape. The actual experiment is very tiny: a flowing liquid sheet only a fraction of a millimeter thick containing a bi-metallic organic complex is exposed to overlapping laser and x-ray pulses in an area much less than a square millimeter.