must

Molecular Ultrafast Science and Technology

Watching molecules and electrons at work

Measuring the fastest processes in nature

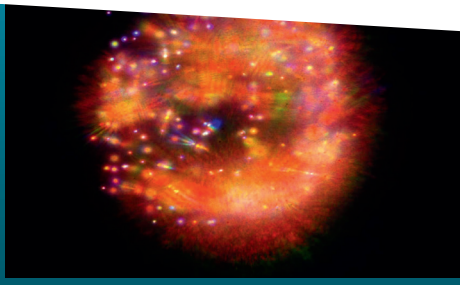
Controlling atomic and electronic motion

National Center for Competence in Research

www.nccr-must.ch

The NCCR MUST is an interdisciplinary research program launched by the Swiss National Science Foundation in 2010. It brings together 18 Swiss research groups working in Ultrafast Science across the fields of physics, chemistry, material sciences and biology.

Scientists have always relied on images of things invisible to the naked eye to advance their scientific knowledge. Seeing things, or visualizing a course of events, is one of the most powerful methods for unraveling nature's secrets. MUST researchers are at the forefront developing new methods and equipment, and using them to study fundamental processes and functions in nature.



Watching molecules and electrons at work

The microscopic structure of molecules and solids is determined by the geometrical arrangement of the different atomic nuclei and the electronic charge densities surrounding them. Without a clear picture of this structure it is hard to understand its function, which is why Francis Crick, the co-discoverer of the double-helix DNA structure, once stated "... If you want to understand function, study structure… ".

Exploring the structure requires tools that can visualize the position and identity of all atoms contained in a molecule or a solid. For example, X-ray crystallography produces three-dimensional images of the electron density, from which this information can be deduced, and reveals information on chemical bonds, disorder and many other properties.

Often, however, the static structure is not sufficient information to work out how a molecule or a solid behaves. Here it is necessary to study the molecules or solids "in action", that is, we must record movies of their evolving structure. To rephrase Francis Crick's original statement "... If you want to understand function, study time-dependent structure… ", which has become the motto of the NCCR MUST.

Observing the fastest processes in nature

The time scale for nuclear motion ranges from femtoseconds (1 femtosecond = 10-15 or 0.000'000'000'000`001 seconds) for elementary processes, in particular photochemical processes, to seconds or even longer for many biological processes. Processes involving electronic motion or the rearrangement and relaxation of an electronic excitation following the absorption of a photon are even faster, often taking only attoseconds (10-18 or 0.000'000'000'000'000'001 seconds), and are highly challenging to observe.

Femto- and attosecond processes can only be visualized through stroboscopic illumination, which requires pulses even shorter than the fastest events under investigation. This became feasible only after the invention of the laser: the only light source capable of producing pulses short enough to record nuclear and electronic motion in real time. Today, MUST-researchers use such ultrashort light pulses throughout a large part of the electromagnetic spectrum, i.e. from THz radiation to X-rays.

Controlling atomic and electronic motion

Conceptually, it is only a small step from observing a nuclear or an electronic motion to controlling it. However, control requires substantially higher light intensities, which is not always easy to achieve. Nevertheless, this avenue is worthwhile pursuing because control over nuclear or electronic dynamics means to take control over the molecule's function. MUST researchers employ different means for control, such as catalysis on surfaces or tailored ultrafast light pulses as so-called "photonic reagents".

Theory and simulations

Research within the NCCR MUST relies on a close interplay between theory and experiment. Several theory groups simulate the dynamics of nuclei and electron densities on different levels of complexity, ranging from classical molecular dynamics simulations to full quantum-dynamical models. They either verify and help understanding experimental observations, or predict microscopic behavior that is later confirmed by experimentalists.

MUST partner institutes and principal investigators

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  Co-director: Thomas Feurer (University of Bern)
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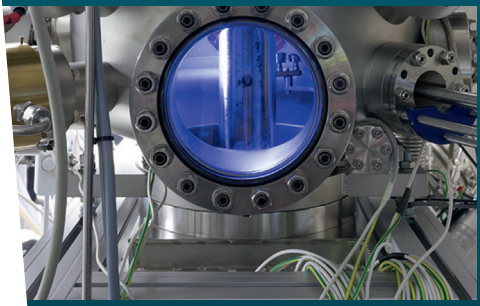
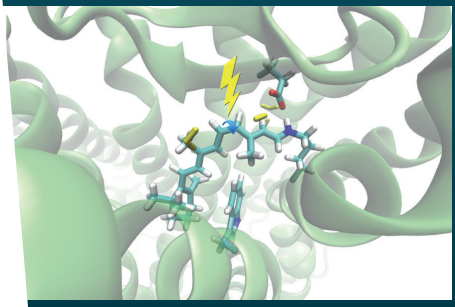
- University of Bern (Co-leading house): Andrea Cannizzo, Thomas Feurer
- EPF Lausanne: Fabrizio Carbone, Majed Chergui, Jacques E. Moser, Ursula Röthlisberger, Jiri Vanicek
- Paul Scherrer Institut: Paul Beaud, Chris Milne, Hans Sigg, Urs Staub,
- University of Zürich: Peter Hamm, Matthias Hengsberger, Jürg Osterwalder
- University of Geneva: Jean-Pierre Wolf
- University of Basel: Markus Meuwly
- University of Neuchatel: Thomas Südmeyer

FNSNF
Swiss National Science Foundation





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