Editorial

National Center of Competence in Research: Molecular Ultrafast Science and Technology

Optical, atomic, and molecular sciences have always had a dramatic impact on fundamental science as well as on our society. They enabled the development of the laser, they triggered the development of quantum mechanics, they are at the heart of modern communication, they facilitate modern navigation systems, they help designing new drugs, or they play a key role in understanding molecules which determine the function of all living creatures. Research efforts in optical, atomic, and molecular sciences are still growing and are expected to have further impact on fundamental sciences as well as our daily life. Francis Crick, the co-discoverer of the double-helix DNA structure, once said "... If you want to understand function, study structure ..." To the present day, the best probes of equilibrium atomic structure in matter are nuclear magnetic resonance, electron spin resonance, high-energy electron scattering, X-ray scattering and X-ray absorption spectroscopy. Especially X-ray scattering has proven to be extremely powerful in unraveling the structure of large molecules, and, unlike any other field, research related to X-rays has been awarded with 19 Nobel prizes in chemistry, physics, and medicine. Time, however, is missing in Francis Crick's statement, but is fundamentally important for chemical reactions, isomerization, or structural phase transitions where a sequence of events of structural and electronic modifications at the molecular level are essential for the understanding of the process. In other words we should probe time-dependent structures and redistribution of electronic charge. Thus, a full understanding of structural dynamic at the molecular level requires a thorough description of the electronic dynamics as the underlying driving force. We have now reached a point where not only do we have the time resolution to probe the motion of atoms within assemblies (molecules, solids, liquids, proteins) but also that of the electrons, which are the main actors in the formation and breaking of bonds.

Over the past years, research along these lines has dramatically gained momentum in Switzerland with new research groups being established, with the implementation of new theoretical concepts, with the development of new sources of femto- and attosecond pulses in the soft and hard X-ray regimes, or with the implementation of various schemes of multidimensional spectroscopy. The Paul Scherrer Institute (PSI) successfully operates the FEMTO facility at the SLS providing hard X-ray pulses of approximately 100-fs duration and plans to further extend its focus in ultrafast science with a new hard X-ray free electron laser (SwissFEL), foreseen to be commissioned by 2017. The aim of MUST is to further promote these developments and to use them in tackling various fundamental problems in molecular sciences by bringing together Swiss researchers active in the development and use of structure-sensitive ultrafast probes. The scientific questions addressed within MUST are focused on increasing our understanding of, and ultimately control of, matter at the level of atoms and electrons. Understanding matter on the atomic scale will address important challenges facing humanity including development of alternative sources of energy and improving health. To address these challenges we need to use and develop new tools that extend into higher spatial, temporal, and energy resolution to visualize and control both atomic and electronic motion in atomic compounds.

Visualization of atomic motion in atomic compounds: The time scale for atomic motion is in the range of femtoseconds to picoseconds and visualization relies on probing techniques which are even faster. Capturing in 'real-time' the motion of atoms, or groups of atoms, in molecules, liquids, solids, and proteins became possible with the advent of femtosecond lasers delivering ultrashort pulses in the ultra-violet, visible, or infrared part of the spectrum. Recently, a major breakthrough has been the development of multi-dimensional spectroscopy in the infrared and, even more recently, in the visible and UV. These optical multi-dimensional spectroscopy techniques are analogues of NMR spectroscopy, with the major advantage that sub-ps temporal resolution is reached (NMR is limited to microseconds at best). Furthermore, couplings between electric dipoles are orders of magnitudes larger than those between magnetic dipoles in NMR, which implies a huge increase in sensitivity. In addition to the progress in transferring NMR-like techniques to the ultrafast domain, X-ray and electron diffraction and X-ray absorption spectroscopy are reaching the relevant time scales. Major breakthroughs in probing ultrafast structural dynamics of chemical and biological systems as well as nano-systems and materials become accessible through ultrashort X-ray and electron pulses. Within MUST, we want to push the development of ultrafast multi-dimensional spectroscopy, of ultrafast X-ray and electron diffraction, and of X-ray absorption spectroscopy as highly sophisticated tools to follow the temporal evolution of structural rearrangements within matter of various sizes and in different environments. Experimental efforts will be accompanied by theoretical work, and we expect that theoretical simulations will help designing appropriate experiments.

Visualization of electronic motion: The time scale of electron motion on a molecular scale is that of attoseconds. Attosecond pulses and novel streaking methods using carrier envelope offset phase-stabilized laser pulses of few optical cycles are available in university-based table-top laboratories and are typically in the VUV to soft X-ray range. They are starting to allow for measurements reaching attosecond resolution for probing electron dynamics in atomic and molecular systems, such as the study of Auger processes, tunneling in atoms, or molecular tomography.

Control of atomic motion in atomic compounds: Control of molecular processes through catalysis on surfaces is a well established method and is omnipresent in our daily life. Steady progress in surface- and nano-science will create a better understanding of such processes and help to devise new ones. Coherent control through optical pulse shaping techniques has been a major area of femtosecond spectroscopy since its birth and in a recent report from the US Department of Energy (*Physics Today*, July 2008 issue) it was identified as one of the most promising and attractive challenges for future research. MUST will increase its already strong efforts in optical pulse shaping and control will also be an integral part of many of the experimental investigations envisaged, as it can help in disentangling complicated measurements.

Already today we witness the benefits of ultrafast science and technology for society and they would not have been possible without the efforts in fundamental research. For example femtosecond lasers are now commonly used in ophthalmology or in confocal microscopy of biological systems; they enable higher accuracy for frequency metrology; they facilitate table-top hard X-ray sources that are being implemented in phase-contrast micro-imaging of biological samples or in high contrast radiography and mammography; they are also used in the processing and machining of solid materials and surfaces as well as in laser-assisted fabrication of new materials. In the future the extension of NMR-like techniques to the infrared and visible spectral domain promises a tremendous leap forward in applications similar to those of NMR, *e.g.* structural determination of molecular systems. Ultrafast spectroscopic measurements will help to better understand the photo-generation of hydrogen, the catalyzed reduction of oxygen, and the charge transfer reactions at the water-supercritical carbon dioxide interface, crucial steps in the upcoming energy problem. Ultrafast spectroscopy will help to understand the dynamics of light-induced electron transfer processes in supra-molecular systems and at interfaces; both being fundamental to the development of dye-sensitized solar cells and resulting photovoltaic systems.

Through MUST we envision advance of knowledge in order to further improve the quality of daily life. New enabling technological innovations will help to further maintain competitiveness and to create new jobs. A major goal of MUST is to provide training and education of qualified personnel and to promote the scientific education of the general public.

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Thomas Feurer was born in Kempten, Germany, in September 1963. He received his Diploma in Physics from the University of Wuerzburg, Germany in 1990. He then moved to the Rice University in Houston, Texas, where he worked on optically induced percolative phase transitions. He earned his PhD degree in Physics in 1994 at the University of Wuerzburg. In 1994 he went to the University of Jena and worked on ultrafast linear and nonlinear optics, femtosecond spectroscopy and coherent control of quantum systems, high-power short-pulse laser-matter interaction at relativistic intensities, generation of femtosecond hard X-rays and femtosecond time-resolved X-ray diffraction. He received the Habilitation in 2001 and moved to the M.I.T. in Cambridge, USA. His research interests were: High-frequency acoustic spectroscopy, ultrafast optics and pulse-shaping, nonlinear spectroscopy of liquids and solids, coherent control of collective excitations in solids, generation of phase-matched high harmonics, EUV nonlinear femtosecond spectroscopy. In 2002 he was appointed Research Associate at the M.I.T. and in 2004 he became full professor at the University of Bern, Switzerland. His current research interests are in ultrafast lasers and fiber optics, ultrafast coherent control and nonlinear spectroscopy. He has published more than 80 journal papers and holds several patents. In 1997, he received the Carl Zeiss Research Award, in 1999 the Werner-von-Siemens Medal, and in 2001 he was awarded with a Max-Kade Fellowship. Thomas Feurer is a member of the Optical Society of America (OSA) and the American Physical Society (APS).

Ursula Keller joined ETH as professor of physics in 1993. She received the PhD in Applied Physics from Stanford University in 1989 and the Physics diploma from ETH in 1984. She was a Member of Technical Staff (MTS) at AT&T Bell Laboratories in New Jersey from 1989 to 1993. Her research interests are exploring and pushing the frontiers in ultrafast science and technology: ultrafast solid-state and semiconductor lasers, frequency comb generation and stabilization, attosecond pulse generation and science using high harmonic generation. She has published more than 310 peer-reviewed journal papers and 11 book chapters and she holds or applied for 17 patents. She received the OSA Fraunhofer/Burley Prize in 2008, the Philip Morris Research Award in 2005, the first-placed award of the Berthold Leibinger Innovation Prize in 2004, and the Carl Zeiss Research Award in 1998. She is an OSA Fellow and an elected foreign member of the Royal Swedish Academy of Sciences and the German Academy Leopoldina.

It is with great pleasure that the Editorial Board of CHIMIA warmly thanks Prof. Dr. Eric Vauthey and his fellow guest editors Prof. Thomas Feurer and Prof. Ursula Keller for their efforts in the planning and successful realisation of this interesting and topical issue on ‘NCCR MUST: A New Swiss Research Priority in Molecular Ultrafast Science and Technology’