gas phase systems with femtosecond temporal resolution to watch even the fastest atomic motions. Some of the important scientific problems to be addressed with ultrabright electron sources will be discussed to give an impression of the potential impact of this emerging field.

[1] B.J. Siwick, J.R. Dwyer, R.E. Jordan, R.J.D. Miller, *Science* **2003**, *302*, 1382-1385. [2] G. Sciaini, M. Harb, S.G. Kruglik, T. Payer, C.T. Hebeisen, F-J. Meyer zu Heringdorf, M. Yamaguchi, M. Horn-von Hoegen, R. Ernstorfer, R.J.D. Miller, *Nature* **2009,** *458,* 56-59. [3] R. Ernstorfer, M. Harb, C.T. Hebeisen, G. Sciaini, T. Dartigalongue, R.J.D. Miller, *Science* **2009,** *323,* 1033-1037. [4] M. Eichberger, H. Schäfer, M. Krumova, M. Beyer, J. Demsar, H. Berger, G. Moriena, G. Sciaini, R.J.D. Miller, *Nature* **2010,** *468,* 799-802.

Keywords: femtosecond electron diffraction, ultrafast structural dynamics, electron sources

MS.45.2

Acta Cryst. (2011) A**67,** C108

Measuring femtosecond structural dynamics at a hard X-ray laser: challenges and successes

David M. Fritz,[a] Henrik Lemke,[a,b] Diling Zhu,[a] Marco Cammarata,[a] [a]*SLAC National Accelerator Laboratory, Menlo Park, California (USA).* [b]*Niels Bohr Institute, University of Copenhagen, Copenhagen (Denmark).* E-mail: dmfritz@slac.stanford.edu

The World's first hard X-ray laser, the Linac Coherent Light Source (LCLS), is now operational at the SLAC National Accelerator Laboratory [1]. The LCLS routinely produces femtosecond pulses of 9 keV photons with 2 mJ of pulse energy at a 120 Hz repetition rate. The unprecedented combination of photon flux, spatial and time resolution of the LCLS promises to revolutionize the observation of structural dynamics by measuring the time evolution of the electron density during a photo-induced transformation.

Although many of the attributes of X-ray laser are ideal for studying structural dynamics, there are significant experimental challenges involved that must be overcome before successful experiments are realized. Unlike storage ring based sources, X-ray pulses from the LCLS exhibit inherent fluctuations due to the self-amplified spontaneous emission (SASE) process through which the radiation is generated. As such the spatial, spectral, temporal and intensity properties vary on a pulse-by-pulse basis. These fluctuations are particularly problematic for experiments studying stimulated dynamics.

The first hard X-ray experimental station, the X-ray Pump-Probe (XPP) instrument, began user operations in the Fall of 2010. The XPP instrument is designed specifically for time-resolved studies and includes a synchronized optical laser. The first experiments included time resolved studies of optically initiated ferroelectricity, photoactive proteins (myoglobin) and iron spin crossover complexes. Many challenges associated with a SASE based X-ray source were encountered. However, most challenges were overcome and a time resolution of 150 fs was achieved.

[1] P. Emma et al., *Nature Photon.* **2010**, *4*, 641647.

Keywords: instrumentation, laser

MS.45.3

Acta Cryst. (2011) A**67,** C108

Structural dynamics of proteins conformers and conformer selection in chemical reactions

S. Techert,[a] M. Petri,[a] M. Scholz,[a] W. Quevedo,[a] M. Wulff,[b] A. Menzel,[c] P. Wernet,[d] A. Foehlisch,[d] [a]*Max Planck Institute for Biophysical Chemistry, IRG Structural Dynamics of (bio)chemical Systems, Goettingen, (Germany).* [b]*ESRF, Grenoble, (France)* [c]*SLS, Villigen, Swiss,* [d]*Helmholtz Center, Berlin, (Germany).* E-mail: stecher@gwdg.de

Characteristic for all chemical reactions are bond breaking and bond making processes. Our vision is to optimize chemical reactions towards specific product states by a clever combination of chemical site-specificity, self-assembly and state-selectivity which can be "tuned" from orbital control through the structure of the local environment and selective excitation schemes (heat / optical pulses) to bulk structural changes – or to say it in other words – from the simple to the complex. We would like to understand - what are the driving forces of environment tuning chemistry? Most motors are defined through gradients in the chemical potential. Are chemical redox potential changes or the changes of chemical potential the most efficient chemical ways for storing energy?

To do so we need to gain a deeper understanding of the mechanism of chemical reactions from a structural point of view – besides its understanding of energetic. In order to elucidate information about reactions and their pathways multidimensional reaction landscapes are required for their description – not only in the energy coordinate but also in the reaction coordinate. In order to elucidate information about the reaction coordinate of complex systems we apply time-resolved x-ray techniques allowing us to obtain a real-time picture of the structural dynamics of chemical and biochemical systems in the crystalline and in the liquid phase.

Common for all time-resolved x-ray experiments is the applied pump / probe scheme, where an optical pump-laser initiates a reaction whose structural time evolution is then investigated by x-ray probe pulses at various time delays. The x-ray photon-in / photon-out techniques are based on diffraction or spectroscopic techniques like near edge spectroscopy or x-ray emission spectroscopy. Meanwhile x-ray spectroscopic techniques probe the local environment around specific atoms in a molecule such as orbitals, crystallographic experiments (monochromatic or Laue) reveal the structure of the bulk of periodic systems. Time-resolved diffuse x-ray scattering experiments give information about the structure of liquids.

In the current contribution we will present our latest efforts in that respect. We will reflect capabilities and limitations of state-of-the-art x-ray techniques for the investigation of two different kind of chemical reactions in complex environment: addition reactions in the solid state and dissociation reactions in the liquid state. We will discuss our current status in reaching this goal (proof-of-principle experiments with free electron laser radiation [1], [2]) and how the investigation of chemical reactions benefits from pulsed synchrotron radiation and Free Electron Laser science as they have been performed at the FLASH facility and at LCLS.

[1] I. Rajkovic et al., *Phys. Rev. Lett.* **2010,** *104,* 125503-6. [2] J. Hallmann, et al., *J. Phys.* **2010,** *B 43,* 194009-194016.

Keywords: FEL research, ultrafast chemistry, structural dynamics

MS.45.4

Acta Cryst. (2011) A**67,** C108-C109

Single-pulse laue TR diffraction: Methods, results and use of QM/MM theory

Philip Coppens, Jason B. Benedict, Anna Makal, Elzbieta Trzop Jaroslaw Kalinowski and Jesse Sokolow. *Department of Chemistry, University at Buffalo-SUNY , Buffalo, NY 14260-3000, (USA).* E-mail: coppens@buffalo.edu