



# Colloquium

**27<sup>th</sup> April 2012 - 13:15**  
**FLASH HALL, Seminar Room (28c)**

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### Structural dynamics from the atom to the scaffold

Our research focusses on the photoinduced structural dynamics of chemical and biological systems in solutions. For this, we use X-ray absorption spectroscopy (XAS) that reports both on the electronic structure (via the pre-edge bound-bound core transitions) and the geometric ones (via the so-called above-ionization XANES and EXAFS features), which we use with picosecond to femtosecond resolution.<sup>1,2</sup> For the study of biological systems, which have very low concentrations, we have developed a new scheme for optical pump/X-ray probe experiments at MHz acquisition rates.<sup>3</sup> We will present our results on nitrosylmyoglobin (MbNO) in physiological solutions, where we identify the docking site of the NO ligand after photodetachment.

However, a full understanding of protein dynamics requires probing the response of the amino acids. For this we implemented 2D transient absorption (TA) spectroscopy around 300 nm which is the absorption region of amino acid residues (e.g., tryptophan). The use of 2D UV TA rather than the more common Fourier transform 2D spectroscopy (FT-2D) is that it ensures a larger bandwidth (~100 nm) than the latter (~10 nm), which is a requirement for biological samples. After demonstrating the performance of the setup on the UV dye 2,5-Diphenyloxazol (PPO) dissolved in cyclohexane, we will present our first results on metMyoglobin and on cyanomyoglobin (MbCN), which represent model systems for the study of MbNO.

1 Femtosecond XANES Study of the light-induced spin crossover dynamics in an Iron(II)-complex Ch. Bressler et al, Science 323 (2009) 489.

2 Probing the transition from hydrophilic to hydrophobic solvation with atomic scale resolution V.-T. Pham et al, JACS 133 (2011) 12740.

3 A high-repetition rate scheme for synchrotron-based picosecond laser pump/x-ray probe experiments on chemical and biological systems in solution F. A. Lima et al, Rev. Sci. Inst. 82 (2011) 063111.