SYSR 1 Hauptvortrag

Zeit: Samstag 08:30–09:00 Raum: TU HE101

Hauptvortrag

SYSR 1.1 Sa 08:30 TU HE101

Transient structures in chemical reactions determined by picosecond x-ray diffraction — •Michael Wulff — European Synchrotron Radiation Facility, Grenoble Cedex 38043, FRANCE

The excited-state structure of small molecules in solution has been studied by combining ultrafast laser techniques with x-ray diffraction. The experiments are done using the pump and probe method: ultra short laser pulses excite a subset of molecules in the sample and delayed x-ray pulses (100 ps) record the structure at a given delay. The diffraction patterns are recorded on a CCD detector in pairs *with* and *without* excitation. The change in the intensity δS(q,t) is then Fourier transformed to δS[r,t], the real-space image of the excited system. There are two contributions to δS[r,t]: the *change* in intramolecular structure of the solute in its cage and the *change* in intermolecular structure in the bulk liquid. We have studied these phenomena for some simple photo reactions in liquids: the dissociation and recombination of I_2 [1], HgI_2, $C_2H_4I_2$ and Br_2 in polar and non-polar liquids. The experimental data will be compared to Molecular Dynamics simulations and we will discuss methods to separate the two contributions.

Finally we will discuss our myoglobin project, specifically the migration of CO in native myoglobin and in the mutant L29F. In both cases the difference maps show how CO moves away from the binding site in jumps between cavities in the protein [2].

[1] A. Plech et al., Phys. Rev. Lett. 92 (2004) 125505; S. Rice, Nature 429 (2004) 255.
[2] F. Schotte et al., Science 300 (2003) 1944.