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Light induced structural changes in photosynthetic reaction centres. Gergely Katona[a], Annemarie Wöhri[b], Linda C. Johansson[a], Emelie Fritz[b], Erik Malmerberg[a], Magnus Andersson[b], Jonathan Vincent[c], Mattias Eklund[c], Marco Cammarata[d], Michael Wulff[d], Jan Davidsson[c], Gerrit Groenhof[e], Richard Neutze[a].
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Photosynthetic reaction centres are responsible for the conversion of light energy to chemical energy in purple bacteria. These membrane proteins contain a special bacteriochlorophyll dimer, two accessory bacteriochlorophylls, two bacteriopheophytins and a statically bound quinone molecule. On the cytoplasmic side, a binding site for a mobile ubiquinone can be located, which is reduced stepwise following light induced charge separation events.
Using continuous illumination we were able to trap a light induced conformational substate at low temperature that develops in response to prolonged intense illumination.[1] This conformational change mainly affects the H-subunit and proposed to play a role to prevent futile charge recombination.
More recently we studied a light induced structural change by Laue diffraction techniques in a related photosynthetic reaction center from *Bl. viridis*.[2] The time-resolved pump-probe experiments were performed at the ID09 beamline of the ESRF using narrow band polychromatic ("pink") X-ray pulses. Laue diffraction images were recorded before and following light activation (3 ms delay) with multiple crystal orientations, until highly complete data was obtained.
In these experiments we observed that residue Tyr-L162 moves closer to the special pair upon illumination which we interpreted as the electrostatic attraction between the positively charged special pair and the deprotonated tyrosine residue. This subtle conformational change highlight the diverse roles tyrosine residues play in various photosystems.

[1] Katona G., Andréasson U., Gourdon P., Snijder A., Hansson Ö., Andréasson L.-E. & Neutze R. *Nat. Struct. and Mol. Biol.* 2005, 12(7), 630. [2] Wöhri A.B., Katona G., Johansson L.C., Fritz E., Malmerberg E., Andersson M., Vincent J., Eklund M., Cammarata M., Wulff M., Davidsson J., Groenhof G. & Neutze R. *Science* 2010, 328, 630.

Keywords: time-resolved crystallography, membrane protein, Laue diffraction, photosynthesis

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Probing catalysis in real time with time resolved x-ray spectroscopy. Matthias Bauer, Jan-Dierk Grunwaldt. *Inst. Für techn. Chemie und Polymerchemie, Karlsruhe Institut für Technologie KIT – Campus Süd, Engesserstraße 18, 76128 Karlsruhe, Germany.*
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X-ray spectroscopy offers many powerful techniques to study catalysts at work. Depending on the catalytic reaction and the scientific question, time and/or spacial resolution is necessary. With the present contribution, the possibilities of X-ray absorption spectroscopy to approach the different time-scales from hours to milliseconds, needed to study heterogeneous and homogeneous catalytic reactions of various experimental requirements are discussed with selected examples, in which also the combination with other spectroscopic methods is highlighted. As such examples will serve: the heterogeneous catalytic partial oxidation of methane and the reduction and re-oxidation of Cu/Al2O3, and the homogeneous cerium catalyzed hydroxylation of diketons as well as the copper-catalyzed Kharash-Sosnovsky reaction.
In both the heterogeneous and homogeneous case, mostly the quick scanning EXAFS technique (QEXAFS) has been successfully applied at the synchrotrons ANKA, APS and SLS, whereas the dispersive EXAFS technique (DEXAFS) was used at the ESRF. In addition we show the importance of complementary techniques like XRD and Raman/UV-Vis spectroscopy as available for example at the Swiss-Norwegian Beamline at the ESRF, in order to understand the total oxidation of methane over Pd/ZrO_2 catalysts and the iron-catalyzed Michael addition.

Keywords: X-ray absorption, Catalysis, Time-resolution

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Chemical reactions of small molecules in solution studied by ultrafast (ps) X-ray scattering. Qingyu Kong[a], Michael Wulff[b], Hyotcherl Ihee[c], Michel H. J. Koch[d]. [a]*Société civile Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin - BP 48, 91192 GIF-sur-YVETTE CEDEX.* [b]*European Synchrotron Radiation Facility, 6 Rue Jules Horowitz, BP220, F-38043 Grenoble Cedex, France.* [c]*Center for Time-Resolved Diffraction, Department of Chemistry, Graduate School of Nanoscience & Technology (WCU), KAIST, Daejeon, 305-701, Republic of Korea.* [d]*European Molecular Biology Laboratory, Hamburg Outstation, EMBL c/o DESY, Notkestrasse 85, D-22603 Hamburg, Germany.*
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Reaction dynamics are traditionally studied by time-resolved spectroscopy employing picosecond or femtosecond optical pulses, in which a reaction is initiated by an optical pulse (pump) and its dynamics is monitored by another optical pulse (probe) at different time delays between the pump and probe pulses. The limitation of optical pump-probe spectroscopy is that the optical pulse only interacts with the outer shell electrons (valence electrons) and the spectroscopic signals are sensitive to only specific energy states, achieving a nanometer resolution. Hard X-rays from synchrotron radiation with a