SFB 1078

Protonation Dynamics in Protein Function

# Colloquium

Mon, **Nov. 18**, 2013 ▪ **14:30 – 16:30** ▪ Lecture Hall B of the Physics Dept. at Freie Universität Berlin (Arnimallee 14, 14195 Berlin-Dahlem)

**14:30** **Prof. Stefan Weber**, Albert-Ludwigs-Universität Freiburg, Germany

***New insights into nitrogenase and flavin-based photoreceptors from EPR***

The bacterial enzyme nitrogenase is able to catalyse the chemical reaction of $N_2$ to ammonia. One of the two metal centers in the MoFe protein of the nitrogenase complex, the FeMo cofactor [7Fe-9S-Mo-X-R-homocitrate], represents the active site of nitrogen reduction. Stefan Weber will present a reinvestigation of highly $^{13}C/^{15}N$ enriched MoFe protein samples using pulsed EPR leading to the proposition that the central atom X is a carbon. He will also give an overview on his recent studies of transient paramagnetic states in blue-light active flavoproteins, such as cryptochromes, phototropins, and BLUF domains.

15:20 Coffee break

**15:40** **Prof. Matthias Ullmann**, University of Bayreuth, Germany

***The Importance of Being Protonated: Considering the Right Protonation for Analyzing Enzymatic Reactions***

Many if not all enzymatic reactions are strongly influenced by electrostatics and thus by the protonation of active site residues. In his talk, Matthias Ullmann will present some examples of enzymes in which the protonation of the active site residue is crucial for the mechanism. In particular, he will present calculations on the mechanism of Ferredoxin-NADP-Reductase and on the glycyl radical enzymes Glycerol Dehydratase and 4-Hydroxyphenylacetate Decarboxylase.

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