

## Opening Colloquium of the Collaborative Research Center 1078 *Protonation Dynamics in Protein Function*

Mon, **May 13, 2013** • **14:30 – 18:10** • Lecture Hall A of the Physics Dept.  
at Freie Universität Berlin (Arnimallee 14, 14195 Berlin-Dahlem)

### Colloquium Program

#### CRC 1078 - Protonation Dynamics in Protein Function

The Collaborative Research Center (CRC) 1078 "Protonation Dynamics in Protein Function" is a research platform, which was initiated and is coordinated by the Freie Universität Berlin (FU). Participating institutions are the Technische Universität Berlin (TU), the Humboldt-Universität zu Berlin (HU), the Charité - Universitätsmedizin Berlin, and the Leibniz-Institut für Molekulare Pharmakologie (FMP). The CRC is funded by the German Research Foundation (DFG) for a period of initially 4 years (Jan. 2013 - Dec. 2016).

The central research goal of the CRC 1078 is to identify and understand a new key principal in protein science, namely the control and coordination of complex protein function by protonation dynamics. To this end, the CRC comprises 15 research projects led by 19 principal investigators (PIs) with a diverse expertise in physics, chemistry, and biology. The CRC also hosts an Intergrated Graduate School for the advanced training of PhD students.

Spokesperson of the CRC 1078 is Prof. Dr. Holger Dau (FU), and deputy spokesperson is Prof. Dr. Peter Hildebrandt (TU).

# Opening Colloquium of the Collaborative Research Center 1078

## *Protonation Dynamics in Protein Function*

I am very pleased to welcome everybody at the Opening Colloquium of the new Collaborative Research Center 1078; and I am very happy that four excellent scientists have followed our invitation, who have shaped the topical research field that we are pursuing in this CRC.

Surprisingly, the hydrophobic protein interior harbors water molecules - often really a lot (more than 1300 in photosystem II). Based on his seminal work in time-resolved (step-scan) FTIR spectroscopy on bacteriorhodopsin, **Klaus Gerwert** has worked out new ideas how protein-internal water clusters may facilitate proton movements.

Efficient energy conversion in respiration involves the 'pumping' of protons driven by electron transfer reactions. In cytochrome-c oxidase, electrons are moving between cofactors and - without ever coming in close contact - these electrons are driving the transfer of protons against the transmembrane pH difference. This wonder of bioenergetics has been revealed by means of elegant biophysical experiments; **Mårten Wikström** has shaped both, the experimental approaches and the resulting new concepts.

Wiring two nails to a car battery, everybody can split water. However, the energetic losses are tremendous and the intricate 4-electron/4-proton chemistry of heterogeneous water oxidation is ill understood. In biology, the photosystem II (PSII) facilitates efficient light-driven water oxidation and we are coming closer to a full understanding. Regarding the water oxidation chemistry of PSII, **Per Siegbahn** is the leading quantum chemist. Per has developed the currently most elaborate and influential mechanistic model of water oxidation in PSII.

It is known for decades that phytochromes control germination and flowering of plants, but it came as a real surprise when **Jon Hughes** and coworkers discovered phytochromes in photosynthetic microorganisms, namely in cyanobacteria. The discovery of cyanobacterial phytochrome has been the beginning of a new area in phytochrome research, with Jon Hughes playing a key role.

I am very happy to welcome these excellent speakers as well as all members and guests of the CRC 1078 at our Opening Colloquium and the subsequent reception. I wish us all a great afternoon and good start into our joint work.

Best regards,  
Holger Dau

## Colloquium Program

- 14:30 Welcome and Opening**  
*Holger Dau (Spokesman of the CRC 1078), Freie Universität Berlin*
- 14:40 Proton transfer via protein-bound water molecules in microbial rhodopsins**  
*Prof. Klaus Gerwert, Ruhr-Universität Bochum, Germany*  
Protein-bound water molecules are crucial for proton-transfer in proteins. This will be exemplified on the proton-transfer mechanism of the light-driven proton pump bacteriorhodopsin and the bacterial photosynthetic reaction-center. The proton-transfer is elucidated with high spatio-temporal resolution by time-resolved FTIR in combination with x-ray structure analysis and biomolecular simulations.
- 15:25 Proton translocation in cellular respiration**  
*Prof. Mårten Wikström, University of Helsinki, Finland*  
The key principles of proton translocation in cell respiration will be reviewed. Recent progress and remaining problems will be high-lighted.
- 16:10 Coffee break**
- 16:40 Proton transfer in photosystem II and cytochrome oxidase**  
*Prof. Per Siegbahn, Stockholm University, Sweden*  
Full mechanisms for water oxidation in PSII and proton pumping in CcO have been derived based on theoretical model calculations. In this talk, the focus will be on the steps where protons are transferred.
- 17:25 How does phytochrome work?**  
*Prof. Jon Hughes, Justus-Liebig-Universität, Germany*  
Phytochromes are red/far-red photochromic photoreceptors used by plants and many microorganisms to perceive their light environment. Finding out how they work continues to be an exciting area of research with plenty of surprises.
- 18:30 Reception and Get-together**  
in the library of the Physics Dept. (on ground floor in Trakt 3)

