



# PHYSIKALISCHES KOLLOQUIUM

Wintersemester 2011/2012

Montag, 17.10.2011, 12 Uhr c.t. H-NB

## Proton-transfer via Protein-bound Water Molecules

**Prof. Dr. K. Gerwert**

Ruhr-Universität Bochum

How protons migrate via protein-bound water molecules is becoming an emerging research-field in biology, ever since Grothuss proposed the proton transfer along water chains in liquid water in physical-chemistry. High resolution three-dimensional crystal-structures in the protein ground states of proton-pumps and proton-channels revealed internal protein bound water molecules. Recent time-resolved FTIR measurements revealed their dynamics, especially the H-bond changes, and showed how such protein bound water molecules can be actively involved in proton transfer using the light-driven proton pump bacteriorhodopsin (bR) as model system [1]. In the first half of the pumping-cycle protons are released from the internal central proton-binding site to the extracellular site of the protein. The detailed proton transfer via such water molecules involves preordered dangling water, a strong hydrogen-bonded water and most interestingly, a protonated water complex as the proton release group, which we identified for the first time in a protein [2]. Such a protonated water-complex was identified before in liquid water and ice by the nobel-laureate Manfred Eigen and is called therefore "Eigen-cation". In the second half of the pumping-cycle, the central binding site is reprotonated from Asp 96 [1]. In contrast to the release site, the uptake site does not contain a pre-ordered water chain in the protein ground state. However, a transient water chain between Asp 96 and the central binding site evolves in an intermediate of the pumping-cycle on the milli-second time-scale. Thereby the proton is transferred from Asp 96 to the central binding site and the pump is reset [4].

In summary, the emerging paradigm invokes the principle that protein bound water molecules are as functional as amino acids residues [2]. A similar mechanism might apply in other proton transferring-proteins such as the photosynthetic reaction-center [5]. The finding by Eigen in liquid water is now extended by our results from physical-chemistry in liquids to the life-science in proteins.

### References

- (1) Gerwert, K., Hess, B., Soppa, J., Oesterhelt, D., *PNAS* 86, 4943-4947 (1989)
- (2) Garczarek, F., Gerwert, K., *Nature* 439, 109-112 (2006)
- (3) Wolf, S., Freier, E., Potschies, M., Hofmann, E. and Gerwert, K., *Angew. Chem. Int. Ed.*, 49, 6889-6893 (2010)
- (4) Freier, E., Wolf, S., Gerwert, K., *PNAS* 108 (28), 11435-11439 (2011)
- (5) Remy, A., Gerwert, K., *Nature Struct. Biol.* 10, 637-644 (2003)

Einführung: Prof. Dr. R.-J. Dettmar

Die Fakultät lädt alle Interessierten herzlich ein.

Ab 11.45 Uhr Kaffee/Tee im Hörsaal