

SFB
1078



Protonation Dynamics
in Protein Function

Mon, January 20,
2014

14:30 – 16:30

Freie Universität Berlin
Physics Department
Lecture Hall B

(Arnimallee 14, 14195 Berlin-Dahlem)

➤ Colloquium

Invited speakers

➤ **Prof. Marcus Elstner** – Karlsruhe Institute of Technology (KIT) – Germany

Classical Force Field and QM/MM simulations of retinal proteins

In the last years, we have combined ab initio quantum chemistry and density functional theory (DFT) methods with empirical force field and continuum electrostatic methods in so called Multi-Scale approaches. I will present the most recent results on the application of these techniques to retinal proteins. We have studied the structure of Channel Rhodopsin, the mechanisms of color tuning as well as proton transport pathways in Bacteriorhodopsin, using a variety of spectroscopic methods like UV/Vis, IR, Raman, NMR in order to clarify details of the molecular structures, not resolved by experiment.

➤ **Prof. Don Lamb** – Ludwigs-Maximilians-Universität (LMU) Munich – Germany

Pulsed Interleaved Excitation and Single Particle Tracking: Fluorescent Tools for Elucidating the Processes of Life

We have developed different fluorescence based methodologies for investigating biological systems. One is pulsed interleaved excitation (PIE) [1]. I will explain the method and the advantages available when combining it with other advanced fluorescence techniques such as Multiparameter Fluorescence Detection (MFD) [2] and Fluctuation Imaging (FI) [3]. A second method we use to investigate important biological processes is single particle tracking [4]. I will discuss how we use PIE-FI and single particle tracking to elucidate HIV assembly and release.

[1] B.K. Müller, E. Zaychikov, C. Bräuchle, D.C. Lamb, *Biophys. J.* 2005, 89, 3508. [2] V. Kudryavtsev, M. Sikor, S. Kalinin, D. Mokranjac, C.A. Seidel, D.C. Lamb, *ChemPhysChem* 2012, 13, 1060. [3] J. Hendrix, W. Schrimpf, M. Höller, D.C. Lamb, *Biophys. J.* 2013, 105, 848. [4] D.C. Lamb, C. Bräuchle, *Physik Journal* 2007, 6, 39. [5] S. Ivanchenko et al. *PLoS Pathogens* 2009, 5, e1000652. [6] V. Baumgärtel et al. *Nature Cell Biology* 2011, 13, 469.

Coffee and tea are ready at 14:15 and during the break.

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