

SFB  
1078



Protonation Dynamics  
in Protein Function

## ➤ Colloquium

Mon, July 6,  
2015

16:15 – 18:30

Freie Universität Berlin  
Physics Department  
Lecture Hall B

(Arnimallee 14, 14195 Berlin-Dahlem)

➤ **Prof. Philipp Kukura** – University of Oxford, UK

### ***What happens after a molecule absorbs a photon***

Light induced processes fundamentally rely on using electronic motion enabled by photon absorption. Whether photoisomerisation, proton or electron transfer, all cases are not driven by the initial absorbed photon; instead the molecule efficiently converts the obtained energy into the desired dynamics. Responsible are the underlying potential energy surfaces and crossings between them such as conical intersections, a paradigm for the breakdown of the Born-Oppenheimer approximation. Although they are well-understood theoretically, they have remained experimentally largely inaccessible. Philipp Kukura will show how the observation of atomic motion in real-time can provide unique information on molecular dynamics and the associated potential energy surfaces ...

[\[Link to the full abstract\]](#)

➤ **Prof. Massimo Olivucci** – University of Siena, Italy, and Bowling Green State University, Ohio, USA

### ***Electronic progression during the photoisomerization of microbial and vertebrate light-sensing rhodopsins***

The functions of microbial and metazoa rhodopsins are usually triggered by the isomerization of their chromophore C13=C14 and C11=C12 bond respectively. To disclose a possible molecular-level basis for such a selection, multiconfigurational quantum chemistry is used to model the sensory rhodopsin from the cyanobacterium *Anabaena PCC 7120* and compare their simulated isomerizations with that of a vertebrate (bovine) rhodopsin (Rh). The results suggest that the 11-cis chromophore of vertebrate and invertebrate visual pigments as well as of photoentraining pigments has been selected to maximize photoisomerization speed and light sensitivity.

Coffee and tea are ready at 16:00 and during the break from 17:10 – 17:30.

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