

SFB  
1078



Protonation Dynamics  
in Protein Function

Mon, Nov. 9,  
2015

16:15 – 18:30

Freie Universität Berlin  
Physics Department  
Lecture Hall B

(Arnimallee 14, 14195 Berlin-Dahlem)

## ➤ Colloquium

➤ **Prof. Marloes Groot** – Vrije Universiteit Amsterdam, The Netherlands

***How does a protein achieve functionality? and  
Third harmonic generation imaging enables fast, label-free characterization  
of human brain tumors***

Two questions at the forefront of biophysical sciences are biological sensing and energy conversion. Photoactive Yellow Protein is at the cross point of these two topics as it converts light energy into a structural change, in the process of biological light sensing. This bacterial photosensor is an excellent model system to study how a protein achieves such a function and results from visible pump/mid-infrared probe studies on the femtosecond to microsecond timescale focused on the initial ultrafast events in PYP will be presented [...]. In the second half of her talk, Prof. Groot will discuss how to obtain label-free images with sub-cellular resolution in deep tissue using higher harmonic generation. Especially optical third-harmonic generation (THG) provides high-contrast imaging of live brain tissue without the need for fluorescent probes. [...] [\[Link to the full abstract\]](#)

➤ **Prof. Daniel Sebastiani** – Martin-Luther-Universität Halle-Wittenberg, Germany

***Ion mobility in complex hydrogen bond networks from combined ab-initio  
molecular dynamics and kinetic Monte-Carlo simulations***

Prof. Sebastiani and his group propose a novel coupling scheme between first principles or force field based molecular dynamics simulations and a kinetic Monte Carlo protocol in view of simulating long-range/long-time ion conduction in disordered condensed phase systems (e.g. liquids, amorphous systems) as well as ordered crystals. The Ansatz is based on periodically adapting the Monte Carlo topology (i.e. the rate matrix) on the evolution of the molecular dynamics trajectory. First applications to proton conduction in hydrogen bonded systems will be presented.

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

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