SFB 1078

Protonation Dynamics in Protein Function

Colloquium

Mon, **Feb. 11,** 2019

15:15 – 17:30

Freie Universität Berlin
Physics Department
Lecture Hall B

(Arnimallee 14, 14195 Berlin-Dahlem)

Prof. Massimo Olivucci – University of Siena, Italy, & Bowling Green State University, Ohio, USA

Recent progress in automatic rhodopsin modeling and its application to the search for fluorescent rhodopsins

Biologists are intensively using computational methods for investigating molecular-level diversity within protein families. In this lecture, we report on a protocol for the fast construction and automation of relatively simple, but congruous, sets of wavefunction-based QM/MM models of rhodopsins, suitable for the investigation of trends in spectroscopic and photochemical properties. By constructing several models of evolutionarily distant rhodopsins we explore the atomic-level causes of observed or predicted functional diversities and similarities of vertebrate, invertebrate and microbial rhodopsins. We have also applied these models to the search for a highly fluorescent microbial rhodopsin. Combined simulation and experimental studies of two mutants of Anabaena Sensory Rhodopsin with contrasting behavior reveal the effects controlling the fluorescence activity.

Prof. Tobias Kampfrath – FU Berlin & Fritz-Haber-Institut der MPG, Berlin

Ultrafast terahertz spectroscopy: probing and controlling fundamental motions of electrons and molecules in condensed matter

The THz frequency range is attracting increasing interest for both applied and fundamental reasons. On one hand, bit rates in current information technology may soon approach the THz range. Therefore, it is warranted to study the behavior of materials at THz frequencies. This goal is also highly interesting from a scientific viewpoint because its low photon energy (4.1 meV at 1 THz) makes THz radiation an excellent probe of many elementary excitations of solids, for instance lattice vibrations (phonons), conduction electrons and molecular rotation. This talk is supposed to provide an introduction to THz spectroscopy of condensed matter. The goal is to illustrate how ultrashort THz electromagnetic pulses (duration <1 ps) can be used as ultrafast ohmmeters and amperemeters to gain insight into elementary motions of electrons and spins in solids and rotations of molecules in solvents. Finally, it will be discussed how very strong THz electric and magnetic fields (~MV/cm and ~T) can even be used to gain control over such motions.

Coffee and tea are ready at 15:00 and during the break from 16:15 – 16:30. www.sfb1078.de

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