Carl von Ossietzky
Universität
Oldenburg
Institut für PHYSIK

PHYSICAL COLLOQUIUM

INVITATION

Monday, 18.01.2021, 4.15 p.m.,
video conference: https://meeting.uol.de/b/anj-2vc-j6s-fwe

speaks

Prof. Dr. Tatiana Domratcheva

Department of Biomolecular Mechanisms,

Max Planck Institute for Medical Research, Heidelberg, Germany

Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

about

"Charge transfer in light activation of biomolecules studied by quantum chemistry"

The talk will present insights provided by quantum chemistry calculations addressing photodynamics and photochemistry of biomolecules. In particular, the focus will be on intermolecular charge transfer electronic states that constitute a common feature of photoactive biomolecules. Initially, quantum-chemistry calculations were proved useful in elucidating molecular mechanisms of flavin-binding photoreceptor proteins and photoenzymes driven by photoinduced electron transfer. Multiconfigurational methods in this case present the most intuitive approach that predicts the energies detected in spectroscopy experiments as well as electron-transfer rates. Based on such calculations, hitherto unknown photochemical reactions have been proposed and supported by further experimental studies. In analogy to flavoproteins, quantum-chemistry calculations identified intermolecular charge transfer in the proteins activated by double-bond isomerization of their light absorbing chromophore. X-FEL experiments, consistent with the computational prediction, established that charge transfer between strictly conserved electron-donor residues and excited chromophore precedes the ultrafast double-bond twisting in bacteriorhodopsin. The talk will discuss quantum-chemistry applications that may help rationalizing the fundamental role of intermolecular charge-transfer in biological photosensory mechanisms.

All interested persons are cordially invited.

Sgd. Prof. Dr. Ilia Solov'yov