# 第356回触媒化学研究センターコロキウム

## Computational studies of photosensitive flavoproteins: from spectroscopy to understanding functional mechanisms

Prof. Tatiana Domratcheva (Max-Planck Institute for Medical Research)

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（創成科学研究棟4階セミナー室C）

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Photosensory flavoproteins activate phototactic responses, circadian adaptation and even neuronal activity. In recent years, these proteins were extensively used in numerous optogenetic applications and as prototypes for engineering fluorescent probes and biosensors. The sensory function of flavoproteins and the fluorescence lifetime depend on the excited states of the flavin cofactor and on flavins's ability to accept or donate an electron. After crystal structures of photosensory flavoproteins such as LOV, BLUF, cryprochromes and photolyases were determined, computational studies of photoexcitation and electron-transfer dynamics in these proteins became possible. In order to conduct such studies, we developed a complex approach that combines high-level quantum-mechanical calculations of excited states and molecular dynamics simulations. With our approach, we study excitation and fluorecent spectral tuning of flavoproteins (and other large biological chromophores) and also obtain rates of individual electron forward- and back-transfer steps among multiple electron donors and acceptors in photosensory proteins. Eventually we study how these electron transfer steps are combined in order to achieve photoactivation. Three specific topics will be presented in this lecture: spectral tuning of flavoproteins in various redox states, insights in the activation of the BLUF photoreceptor, and characterization of complex electron transfer pathways in DNA repair enzymes photolyases.

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2000, PhD in Chemistry (Prof. Stepanov), Department of Chemistry, M.V. Lomonosov Moscow State University, Russia. Dissertation Title: "Quantum-chemical modeling of water clusters interacting with dehydroxylated zeolites". 2001-2004, Post-doc (Prof. Goody) Max-Planck Institute of Molecular Physiology, Dortmund, Germany. 2004-2009, Research Associate (Wissenschaftliche Mitarbeiter), Department of Biomolecular Mechanisms, Max-Planck Institute for Medical Research, Heidelberg, Germany. 2009, W2 Professor Position awarded by the Minerva Program of the Max-Planck Society supporting women in science. 2009-(present), Leader of the Computational Photobiology Group, Department of Biomolecular Mechanisms, Max-Planck Institute for Medical Research, Heidelberg, Germany. 2015, Visiting professor at Nagoya Institute of Technology supported by "Research Unit Invitation" of NIT.