

**Department Biologie, Chemie, Pharmazie**  
**Institut für Chemie**  
**Project "Computational modeling of blue light pathways in light harvesting complexes"**

**PhD position for 3 years**  
**ID: QC BioSys - 01 - 2018**

Our group "Quantum chemistry of biological systems" investigates a variety of biological targets using state-of-the-art quantum chemistry and force field approaches. Our main task is the investigation of light harvesting proteins and the role of chromophores located within these complexes. We explore possibilities for energy transfer that are not trivial to track in the lab, and we work closely with experimentalists to elucidate pathways that are otherwise not obvious. As such, we are always on the lookout for individuals who are able to handle multiple challenging fields at the same time, among them biology, quantum chemistry and spectroscopy. We cooperate with local, national and international groups to integrate our findings with experimental results.

**Job description:**

Your task will be to investigate the interactions between light harvesting chromophores using density functional theory (DFT) and related methods. You will also study the effect of the protein environment in terms of promoting or suppressing such interactions. To do so, you will employ combinations of quantum mechanics and molecular mechanics (QM/MM), as well as simplified approaches to obtain quantitatively large amount of results. The identified energy transfer pathways will be used as predictions for experiment, and also to obtain model systems that can be treated using dynamic approaches. You will cooperate with local groups to obtain insights on the pathways and their control mechanisms in more ways than could be obtained from the stationary calculations alone. Your results may uncover new functions and roles of biological light harvesting systems, which could lead to enhanced understanding in biomimetic systems for, e.g., energy generation and transfer.

**Prerequisites:**

A masters degree in biochemistry, chemistry, biophysics or a related field is required.

**Additional skills:**

Experience with quantum chemistry software or force field packages; basic knowledge of plant physiology; ability to work autonomously and solving complex problems; at least one programming/scripting language (preferably python or C++)

Applications containing the characteristic documents are to be send in PDF format to Dr. Jan Philipp Götze ([jan.goetze@fu-berlin.de](mailto:jan.goetze@fu-berlin.de)) until **16 April 2018** including the **ID** via email or by post to

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Legal details apply as stated in the official job offer found at <http://www.fu-berlin.de/service/stellen/st-2018/st-20180326/index.html>