SFB 1078

Protonation Dynamics in Protein Function

Mon, **February 08**, 2021

15:15 – 16:15

Freie Universität Berlin

via WebEx

Colloquium

Dr. Dimitrios A. Pantazis

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Excited states of photosynthetic pigments from quantum chemical and multilevel approaches

A range of molecules with conjugated systems, such as chlorophylls, pheophytins, and carotenoids, are utilized by photosynthetic systems to carry out light absorption, excitation energy transfer, and charge separation. The accurate prediction of the excitation energies of the chromophores (or site energies) and the description of the excited states themselves at the quantum mechanical level can be very useful in understanding these fundamental processes. Here I will describe our efforts to approach this problem using modern quantum mechanical methods based on density functional theory as well as on the most recent correlated wave function theory implementations. One particular point of focus will be on the prediction of the effect of the protein matrix on excitation energies, i.e. the protein-induced electrochromic shifts. I will discuss how our work has helped to describe the emergence of excited-state asymmetry in the reaction center of Photosystem II at the quantum chemical level, how it relates to the question of far-red light excitation, and how it is currently being extended to related photosynthetic components and processes.

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