Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Thursday, November 30th , 2017 – 2:00 p.m.
CFEL Seminar room IV | 01.111 | (Bldg. 99)

Thomas Renger

Johannes Kepler University, Linz, Austria
Institute of Theoretical Physics Department of Theoretical Biophysics

Structure-based theory of light-harvesting in photosynthesis

Two challenges in the simulation of excitation energy transfer and optical spectra of pigment-protein complexes are the equal magnitude of the excitonic and the exciton-vibrational coupling and the structure-based parametrization of the Hamiltonian (for review see ref. 1). We have developed quantum chemical/electrostatics/normal mode analysis (NMA) schemes to calculate optical transition energies of pigments in their binding site in the protein (site energies), interpigment excitonic couplings and the spectral density of the pigment-protein coupling. Our NMA of the spectral density shows that the modulation of site energies is an order of magnitude stronger than that of the excitonic couplings and that also in the basis of delocalized exciton states the diagonal exciton-vibrational coupling dominates [2]. This result explains the good performance of our earlier time-local lineshape theory [3], in which the diagonal elements are treated exactly and the off-diagonal elements in Markov and secular approximations, and triggered a new development that takes into account the finite relaxation time of nuclei during exciton relaxation [4]. I will give a summary of our theory development and present applications on a small model system (water soluble chlorophyll binding protein -WSCP) and large photosystem II core particles. In the case of WSCP we have developed and applied a theory of holeburning spectroscopy [5] that goes beyond the standard two-level system approach and allows for a quantitative description of experimental data, revealing the lifetime of the upper exciton state, in excellent agreement with results from 2D electronic spectroscopy and our earlier prediction [6]. In the case of photosystem II I will present results of the parametrization of the exciton Hamiltonian of its subunits [7-9]. These parameters were used to describe VIS/IR pump-probe data on single crystals of PSII core particles [10] that allowed for a verification of our earlier prediction [11] on the relative time-scale of excitation energy and charge transfer in this system. The results are discussed in terms of photoprotection scenarios that allow photosystem II to switch between a light harvesting and an excitation energy quenching mode protecting the reaction center.

References

[1] T. Renger, F. Müh (**2013**) *Phys. Chem. Chem. Phys. 15*, 3348.
[2] T. Renger, A. Klinger, F. Steinecker et al. (**2012**), *J. Phys. Chem. B 116*, 14565.
[3] T. Renger, R. A. Marcus (**2002**) *J. Chem. Phys. 116*, 9997.
[4] T.-C. Dinh, T. Renger (**2016**) *J. Chem. Phys. 142,* 034104.
[5] J. Adolphs, M. Berrer, T. Renger (**2016**) *J. Am. Chem. Soc. 138*, 2993.
[6] T. Renger, I. Trostmann, C. Theiss et al. (**2007**) *J. Phys. Chem. B 111*, 10487.
[7] F. Müh, M. Plöckinger, T. Renger et al. (**2015**) *J. Photochem. Photobiol. B. 152*, 286.
[8] J. Hall, T. Renger, F. Müh, R. E. Krausz et al. (**2016**) *Biochim. Biophys. Acta 1857*, 1580-1593.
[9] F. Müh, M. Plöckinger, T. Renger (**2017**) *J. Phys. Chem. Lett. 8*, 850.
[10] M. Kaucikas, K. Maghlaoui, J. Barber, T. Renger, J. van Thor (**2016**) *Nature Comm*. 7, 13977.
[11] G. Raszewski, T. Renger (**2008**) *J. Am. Chem. Soc. 130*, 4431.

Host: R. J. Dwayne Miller

MAX-PLANCK-GESELLSCHAFT