Monte Carlo Simulation of the Photophysics of Artificial Antennas for Organic Solar Cells

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Porphyrin are interesting building blocks for the construction of very thin films as artificial antenna s, for organic solar cells [1]. Whether an artificial antenna efficiently transports excitation energy is mainly determined by the mechanism and rate of energy transfer between acceptor- and donor layers in the films. Detailed knowledge of the film structure and its aggregated building blocks, its spectroscopic properties, and the nature and strength of the intermolecular interactions at the aggregate and domain level is required to optimize energy transfer throughout the film [2]. With the application to light-harvesting antennas in solar cells in mind the energy transfer and excited state decay properties of artificial antenna s have been investigated by the Monte Carlo (MC) simulation-fitting method [3]. Using this computational technique the complex steady state fluorescence spectra and the fluorescence- and fluorescence anisotropy decay of porphyrin oligomers in solution as well as of thin solid films has been analyzed.

This work focuses on the structure and photophysics of

- zinc mono-(4-pyridyl)-triphenylporphyrin (Zn(4-Py)TrPP) self-organizing into a tetramer $[Zn(4\text{-}Py)TrPP]_4$
- self-organizing zinc tetra(-octylphenyl)-porphyrin (ZnTOPP) layers on an inert substrate.

Films of Zn(4-Py)TrPP and ZnTOPP were made by spincoating from toluene [4]. Steady-state and time resolved spectroscopy show that ZnM(4-Py)TrPP in solution polymerizes to a tetramer through internal zinc-pyridyl ligation (Fig.1) [1]. Preliminary results of MC simulations of ZnM(4-Py)TrPP films agree with this tetramer model, yielding a fluorescence lifetime and nearest neighbor energy transfer rate constant of $\sim 1.5 \times 10^{-9}$ s and $\sim 40 \times 10^{9}$ s^{-1}, respectively. Applying these simulations to the experimental fluorescence- and fluorescence anisotropy decay of ZnTOPP films results in a multi-domain model of parallel porphyrin stacks. In each stack the porphyrin planes are perpendicular to the substrate and form an angle of 45ß with the long stack axis (Fig. 2). MC simulation yields the rate

constants for intra-stack and inter-stack energy transfer as ~ 1×10^{12} s^{-1} and ~ 80×10^{9} s^{-1}, whereas the fluorescence lifetime is ~ 1.8×10^{-9} s.

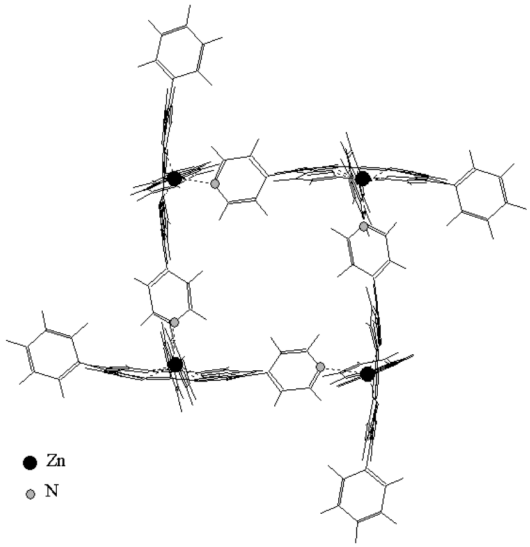

Fig.1. Molecular structure of [Zn(4-Py)TrPP]$_4$

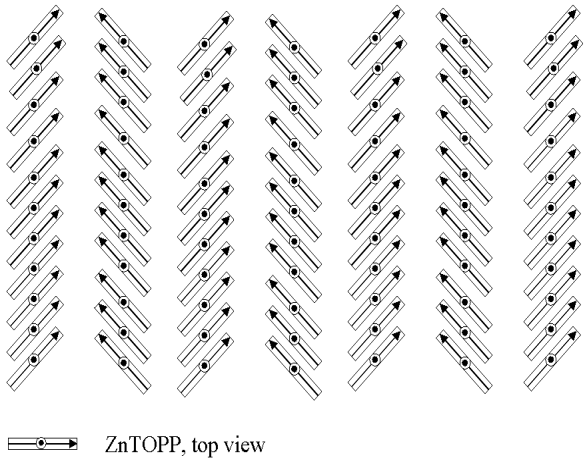

Fig.2. Fragment of ZnTOPP layer on a quartz substrate

The results of this work show that MC simulation of the energy transfer processes in thin films of self-organized [Zn(4-Py)TrPP]$_4$ tetramers and ZnTOPP nanolayers, using a physical model of their structure and excited state kinetics, is a successful method to extract the relevant kinetic parameters from the experimental complex fluorescence and fluorescence anisotropy decay of the film. The MC simulation-fitting method is not limited to the process or system as in this work, but is expected to be equally effective for other more complex artificial antennas systems and/or different processes involving excited states.

References

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