Excitation Energy Transport in Confined Nanoscale Geometries: Theory and Monte Carlo Modeling

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Non-radiative transport of electronic excitation energy, including Förster Resonance Energy Transfer (FRET) and excitation energy migration, plays a key role in the optical properties of nanoscale systems and has numerous applications in bioimaging, biosensing, photonics, and nanotechnology. While classical theoretical models of energy transport were developed mainly for macroscopic and effectively infinite media, their direct application to confined nanoscale geometries is limited.

In this work, theoretical and numerical studies of excitation energy transport in nanostructures of spherical and cylindrical symmetry are presented. Analytical models describing donor fluorescence decay were developed for systems involving Förster-type energy transfer, excitation energy migration within donor ensembles, and combined migration–transfer processes. Particular attention was devoted to hybrid core–shell nanostructures, where chromophores are distributed within the shell volume or attached to the nanoparticle surface.

The proposed models were validated using Monte Carlo simulations based on a step-by-step stochastic algorithm adapted to finite nanoscale geometries. The simulations enabled investigation of the influence of molecular distribution, confinement effects, and geometry on the efficiency and dynamics of excitation energy transport.

The presented results contribute to bridging the gap between experimental studies of nanoscale systems and the theoretical description of excitation energy transport in confined geometries.

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