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The subject of the doctoral dissertation: Photo-induced electron transfer reactions in liquid crystals

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Abstract:

This work aims to describe anisotropy effects on chemical reactions imposed by the structure of liquid crystals. Photo-induced electron transfer reactions of two kinds, namely intramolecular and intermolecular electron transfers, are studied in order to observe the influence of the medium with and without material diffusion. The first kind is studied using a donor covalently linked to an acceptor molecule in many solvents. Two elementary models, based on the Generalized Smoluchowski equation and on the Generalized Langevin equation are applied to explain the time evolution of the fluorescence emission during the adiabatic charge transfer. Once well characterized an attempt to study the same system in liquid crystals is performed. On the other hand, the intermolecular electron transfer reactions are studied using the fluorescence quenching in the excited state. The charge shift and charge separation reactions are investigated in two different chemical systems. The second reaction has molecules resembling the moieties in the intramolecular electron transfer study. Steady state and time resolved measurements are performed to track the reaction kinetics. The reactions are first conducted in isotropic media at different temperatures and viscosities to extract the electron transfer parameters which are independent of the solvent. A set of diffusion-reaction models with different levels of anisotropy has been developed as well as a numerical method to solve the corresponding partial differential equations. Only the model which introduces anisotropic diffusion and reactivity gives physically meaningful values for all parameters entering the reactivity. It is therefore shown how to adapt reaction-diffusion models able to accommodate any sort of reactivity to complex environments.