Modeling Exciton Dynamics in Organic Nanofibers

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Organic nanofibers have been widely investigated both in industry and academy due to their potential applications in optoelectronic devices. The preparation process allows for a fine tuning of their optical properties and strongly depends on its molecular composition. Here we investigate multilayered nanofibers made out of poly(para-phenylene) – P6P and α-sexithiendiy (T6) alternating layers. By means of TD-DFT calculations, we simulated the absorption and emission spectra in these two molecules composing the nanofibers and characterize the Förster transitions on a first step. Later, by means of a Kinetic Monte Carlo (KMC) simulation, combined with a genetic algorithm (GA), we reproduced the time-resolved photoluminescence measurements carried out for different temperatures. This hybrid theoretical-experimental procedure allows for the determination of different information regarding the exciton diffusion in such system, including: (i) the influence of temperature on the Förster transfer efficiency and (ii) the activation energy of the diffusion process. Our model was capable of reproducing experimental measurements and proved to be an efficient tool to describe exciton dynamics in different materials and can be used with different morphologies.

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