Exciton simulations: from liquid crystals to porphyrin-CNT aggregates

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Most organic electronic devices are made of molecular building blocks that self-assemble into non-covalently interacting architectures. These functional materials possess unique photophysical properties and their characterization often requires the development of theoretical models to interpret experimental results.
In this regard, an algorithm[1] for the simulation of exciton dynamics has been implemented and used to reproduce the spectroscopical features of different self-organized systems with applications in organic photovoltaics. The model has been applied to reproduce the spectral features of a substituted oligo(p-phenyleneethynylene) (OPE) liquid crystals[2,3] and an aggregate made of protonated porphyrins (H_4P^{2+}) and carbon nanotubes (CNTs)[4,5].

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