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Monte Carlo Simulation of Exciton Dynamics in Supramolecular Semiconductor Architectures CARLOS SILVA, CLÉMENT DANIEL, University of Cambridge, DAVID BELJONNE, University of Mons - Hainaut, LAURA HERZ, University of Oxford, FREEK HOEBEN, PASCAL JONKHEIJM, ALBERTUS SCHENNING, BERT MEIJER, Eindhoven University of Technology — Supramolecular chemistry is useful to construct molecular architectures with functional semiconductor properties. To explore the consequences of this approach in molecular electronics, we have carried out ultrafast measurements of exciton dynamics in supramolecular assemblies of an oligo-*p*-phenylenevinylene derivative functionalized to form chiral stacks in dodecane solution in a thermotropically reversible manner. We apply a model of incoherent exciton hopping within a Monte Carlo scheme to extract microscopic physical quantities. The simulation first builds the chiral stacks with a Gaussian disorder of site energies and then simulates exciton hopping on the structure and exciton-exciton annihilation to reproduce ensemble-averaged experimental data. The exciton transfer rates are calculated beyond the point-dipole approximation using the so-called line-dipole approach in combination with the Förster expression. The model of incoherent hopping successfully reproduces the data and we extract a high diffusion coefficient illustrating the polymeric properties of such supramolecular assemblies. The scope and limitations of the line-dipole approximation as well as the resonance energy transfer concept in this system are discussed.

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