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Interactions between linear organic chromophores: an improved line-dipole approximation JEAN-CHRISTOPHE DENIS, Institute for Photonics and Quantum Sciences, School of Engineering and Physical Sciences, SUPA, Heriot-Watt University, Edinburgh EH14 4AS, UK, STEFAN SCHUMACHER, Physics Department and Center for Optoelectronics and Photonics Paderborn, Universität Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany, IAN GALBRAITH, Institute for Photonics and Quantum Sciences, School of Engineering and Physical Sciences, SUPA, Heriot-Watt University, Edinburgh EH14 4AS, UK — Modelling accurately the interactions between chromophores is key for realistic simulations of the dynamics of exciton transfer and annihilation in organic semiconductor films. In the framework of Förster theory, it is required to calculate the interaction matrix elements for all relative orientations and separations of chromophores. Therefore a fast and robust approximation is necessary to simulate extended multi-chromophoric systems. From this perspective, using the line-dipole approximation is a very natural approach. However, by a comparative study of the dipole approximation with quantum chemistry (TD-DFT) we demonstrate that the usual line-dipole theory, while successful for short molecules, does not describe well the interactions of longer molecules, where separations are smaller than the interacting chromophores - a limit typically reached in polymer films. As an alternative, we propose an improved way of distributing the sub-dipole moments within a line. This approach remains simple enough to be used in large-scale calculations, while the agreement with the quantum chemistry is significantly improved for all relative orientations.

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