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Photophysics of charge-transfer excitons in thin films of π-conjugated polymers[1] DEMETRA PSIACHOS, SUMIT MAZUMDAR, University of Arizona — We develop a theory of the electronic structure and photophysics of interacting chains of π-conjugated polymers to understand the differences between solutions and films. While photoexcitation generates only the intrachain exciton in solutions, the optical exciton as well as weakly allowed charge-transfer excitons are generated in films. We show that a significant fraction of ultrafast photoinduced absorptions (PAs) in films originate from the lowest charge-transfer exciton. Using sophisticated many-body approaches that take into account high order configuration interaction, we have calculated the full wavelength-dependent PA spectra of pairs of interacting PPV oligomers. Good qualitative agreement is obtained with the experimental PA spectra of thin films of π-conjugated polymers. The origin of each individual PA is explained within our theory. Our work resolves long-standing controversies regarding the nature of the primary photoexcitations in films.

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