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Theory of interfacial charge-transfer complex photophysics in π-conjugated polymer-fullerene blends[1] K. ARYANPOUR, D. PSIACHOS, S. MAZUMDAR, Department of Physics, University of Arizona — We present a theory of the electronic structure and photophysics of 1:1 blends of derivatives of polyparaphenylenevinylene and fullerenes [1]. Within the same Coulomb-correlated Hamiltonian applied previously to interacting chains of single-component π-conjugated polymers [2], we find an exciplex state that occurs below the polymer's optical exciton. Weak absorption from the ground state occurs to the exciplex. We explain transient photoinduced absorptions in the blend [3], observed for both above-gap and below-gap photoexcitations, within our theory. Photoinduced absorptions for above-gap photoexcitation are from the optical exciton as well as the exciplex, while for below-gap photoexcitation induced absorptions are from the exciplex alone. In neither case are free polarons generated in the time scale of the experiment. Importantly, the photophysics of films of single-component π-conjugated polymers and blends can both be understood by extending Mulliken's theory of ground state charge-transfer to the case of excited state charge-transfer. [1] K. Aryanpour, D. Psiachos, and S. Mazumdar, arXiv:0908.0366 [2] D. Psiachos and S. Mazumdar, Phys. Rev. B. **79** 155106 (2009) [3] T. Drori *et al.*, Phys. Rev. Lett. **101**, 037402 (2008)

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Karan Aryanpour
Department of Physics, University of Arizona

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