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Photophysics of MEH-PPV film under High Hydrostatic Pressure: The Role of Charge-Transfer Excitons[1] S. MAZUMDAR, K. ARYANPOUR, D. PSIACHOS, Department of Physics, University of Arizona — We report theoretical calculations for interacting pairs of PPV oligomers that explain the pressure-dependent experimental observations on MEH-PPV films by E. Olejnik *et al.* We use the Pariser-Parr-Pople (PPP) model Hamiltonian for single chains. We assume that pressure decreases the intermolecular distance in the ordered phase of this two-phase material, and simulate pressure effects by assuming distance-dependent interchain Coulomb interactions and electron hopping. Our calculations show that the photophysics of the ordered phase is dominated by a charge-transfer exciton, which is a quantum-mechanical superposition of the covalent delocalized exciton state and the ionic polaron-pair state. We are able to explain the pressure-induced (i) quenching of the photoluminescence and its redshift, (ii) the redshift of the cw triplet photoinduced absorption, (iii) the appearance of ps PA bands at $\sim$ 0.35 eV and 0.9 eV and their strong blueshifts. Detailed comparisons between experiments and theory are made.

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