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Revealing photoinduced charge transfer mechanism across π-conjugated heterojunctions YONGWOO SHIN, XI LIN, Boston University — The adapted Su-Schrieffer-Heeger (aSSH) model is extended to the π-conjugated bulk heterojunction system. The New aSSH Hamiltonian incorporated interchain π-π stacking and dynamic electron-phonon coupling effects. Excellent agreements are found between the computed photoadsorption and photoinduced adsorption spectra and their corresponding experimental measurements. It is found that excitons generated in the bulk poly-(p-phenylene vinylene) (PPV) phase must overcome an energy barrier of 0.23 eV to reach heterojunction interface. These interfacial excitons show clear charge separations, with their electron states leaning towards the interface. Therefore, electron transfers from the D_1^* state of PPV to the t_{1u}^* state of C_{60} follow non-adiabatic mechanisms, which are accelerated by the 0.97 eV energy drop, close vicinity of the D_1^* state to the C_{60} phase, and suppressed inversion symmetry that doubles the number of electron-accepting states. After non-adiabatic electron transfers, the hole D_1 states are screened by the optical phonons in PPV, forming self-localized hole polarons and moving further away from heterojunction interface.

Yongwoo Shin
Boston University

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