

Abstract Submitted
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Driving intramolecular charge transfer by tuning molecular orbitals and dielectric constants MELISSA APLAN, YOUNGMIN LEE, JASON MUNRO, CHRISTOPHER GRIECO, The Pennsylvania State University, ZACH SIEBERS, S. MICHAEL KILBEY, The University of Tennessee, ISMAILA DABO, QING WANG, JOHN ASBURY, ENRIQUE GOMEZ, The Pennsylvania State University — Fully conjugated block copolymers, consisting of an electron donor and an electron acceptor block, can serve as the active layer in organic photovoltaic devices. Incorporating the donor-acceptor interface within the chemical structure enables model studies of energy and charge transfer. We synthesized a series of block copolymers consisting of a P3HT electron donor and a push-pull polymer electron acceptor, either poly-2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopentadithiophene)-alt-[4,7-bis(3-dodecylthiophen-5-yl)-2,1,3-benzothiadiazole]-2',2''-diyl) (PCPDT12BT), poly-((9-(9-heptadecanyl)-9H-carbazole)-1,4-diyl-alt-[4,7-bis(3-hexylthiophen-5-yl)-2,1,3-benzothiadiazole]-2',2''-diyl) (PCT6BT), poly-((9,9-dioctylfluorene)-2,7-diyl-alt-[4,7-bis(3-hexylthiophen-5-yl)-2,1,3-benzothiadiazole]-2',2''-diyl) (PFT6BT), or poly-((2,5-dihexylphenylene)-1,4-diyl-alt-[4,7-bis(3-hexylthiophen-5-yl)-2,1,3-benzothiadiazole]-2',2''-diyl) (PPT6BT). By altering only the electron rich unit of the acceptor, we adjust the energy difference between the HOMO of the donor and acceptor by tenths of an eV. Absorption and emission spectra of the block copolymers enable us to quantify the yield of intramolecular charge transfer states in dilute solutions. We find a critical driving force required to generate CT states that depends on the dielectric constant of the solvent.

Melissa Aplan
The Pennsylvania State University

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