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Suppressing intermolecular charge recombination in photovoltaics through conjugated block copolymer architectures

HAO KUANG, ENRIQUE GOMEZ, MICHAEL JANIK, Department of Chemical Engineering, The Pennsylvania State University

— Block copolymers have the potential to control the interfacial and mesoscopic morphology of the active layer of organic photovoltaics and consequently enhance device performance. For example, the self-assembly of conjugated block copolymers into periodic microstructures with nanometer length scales could facilitate exciton dissociation by creating large amounts of donor-acceptor interfaces. Furthermore, the interfacial structure may strongly affect charge transfer processes. Using Density Functional Theory, we have examined charge transfer rates in model interfaces of poly(3-hexylthiophene)−block−poly-((9,9-dioctylfluorene)-2,7-diyl-alt-[4,7-bis(thiophen-5-yl)-2,1,3-benzothiadiazole]-2′,2?-diyl) donor-acceptor block copolymers which yield 3% efficient devices when incorporated into solar cells. Our results demonstrate that intermolecular charge recombination can depend on the interfacial breadth, where sharp interfaces (ca. 1 nm) suppress intermolecular charge recombination by orders of magnitude. Furthermore, we compare intramolecular and intermolecular charge transfer rates in donor-acceptor block copolymers through Constrained Density Functional Theory calculations.

Hao Kuang
Department of Chemical Engineering, The Pennsylvania State University

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