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Donor-acceptor polymers for organic photovoltaics

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Furan and its derivatives are promising alternative building blocks for the synthesis of semiconducting polymers due to their properties such as smaller heteroatom size, more electronegative heteroatom, and larger dipole moment. Conjugated polymers synthesized from furan show a higher degree of conjugation with reduced twisting between adjacent units, smaller π -stacking distance, and improved solubility in organic solvents. Despite research on polymers constructed from furan derivatives gaining attention, conjugated polymers from furan only are still scarce. We reported a conjugated polymer, poly(4,8-bis(5-(2-ethylhexyl)furan-2-yl)benzo[1,2-b:4,5-b']difuran-alt-2,5-didodecyl-3,6-di(furan-2-yl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione), P(BDF-FDPP), for organic solar cells. The smaller oxygen atom in furan of P(BDF-FDPP) resulted in a planar conjugated backbone with negligible torsion (dihedral angle < 0.10) determined by density functional theory. P(BDF-FDPP) exhibited broad absorption up to 940 nm with HOMO and LUMO located at -5.19 eV and -3.63 eV, respectively. Power conversion efficiency (PCE) of 5.55% with a high fill factor (FF) of 0.73 was measured for the devices fabricated using diphenyl ether (DPE) as an additive. The considerable change in photovoltaic performance of the devices fabricated with or without additives was investigated with grazing incident wide-angle X-ray scattering, and transmission electron microscopy experiments. Preferential face-on orientation of P(BDF-FDPP) and sophisticated interpenetrated network for P(BDF-FDPP)/PC71BM blend films enabled relatively good PCEs and high FF in solar cell devices.

Biography

Mihaela C Stefan received her PhD degree in Chemistry from Politehnica University Bucharest. She joined the Department of Chemistry at the University of Texas at Dallas in 2007 and was promoted to Associate Professor in 2013. She has received a joint appointment in the Bioengineering Department in 2014. She received the NSF Career Award in 2010, the NS&M Outstanding Teacher Award in 2009 and 2017, the Inclusive Teaching Diversity Award in 2012, President's Teaching Excellence Award in 2014, and the Provost's Award for Faculty Excellence in Undergraduate Research Mentoring in 2015. Her research group is developing novel polymeric materials for organic electronics and drug delivery applications.

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