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Development of Wide Bandgap Polythiophene Polymers with Deep-lying HOMO Energy Level and Reduced χ for Improving Photovoltaic Efficiency

B. Advancing sustainable organic photovoltaics: from experiments and materials to applications and device models

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Abstract

In this work, we report a novel set of polythiophene derivatives (**PDC8T**, **PDC8TT**, **PDC16TT**, and **PDC16TF**) featuring carboxylate substitution to fine-tune electronic properties via a simplified three-step synthesis. These derivatives demonstrate a notable decrease in HOMO energy levels by approximately 0.3 to 0.4 eV compared to the benchmark polymer poly(3-hexylthiophene) (P3HT). We employed them in inverted non-fullerene bulk-heterojunction (NFA BHJ) OPVs. Particularly, the fluorinated PT derivative, **PDC16TF**, led the series with an exceptional power conversion efficiency (PCE) of 7.21%, delivering a V_{OC} of 0.846 V, a J_{SC} of 14.60 mA cm⁻², and an FF of 58.4%. Such an improvement is credited to the syngenetic effect of carboxylate and fluorination substitutions which downshift the HOMO level alignment, induce a coplanar conformation, and improve molecular orientation. Besides, the molecular design strategy has culminated in a fibrillar bicontinuous interpenetrating network with optimal phase separation at the nanoscale within the active layer to achieve optimal miscibility.