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Small Molecule Acceptor and Polymer Donor Crystallinity and Aggregation Effects on Microstructure Templating: Understanding Photovoltaic Response in Fullerene-Free Solar Cells.

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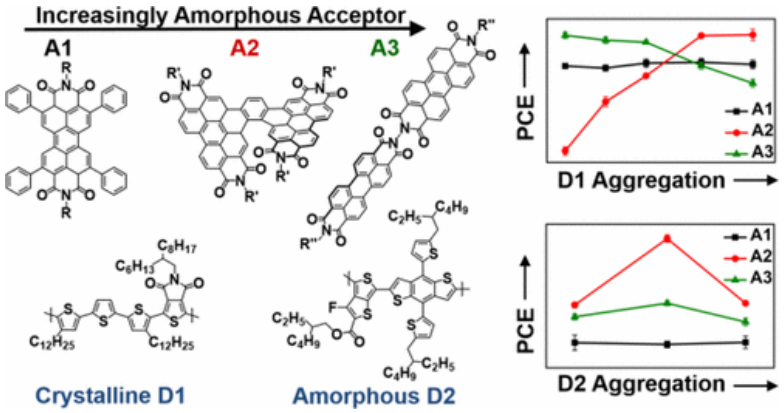
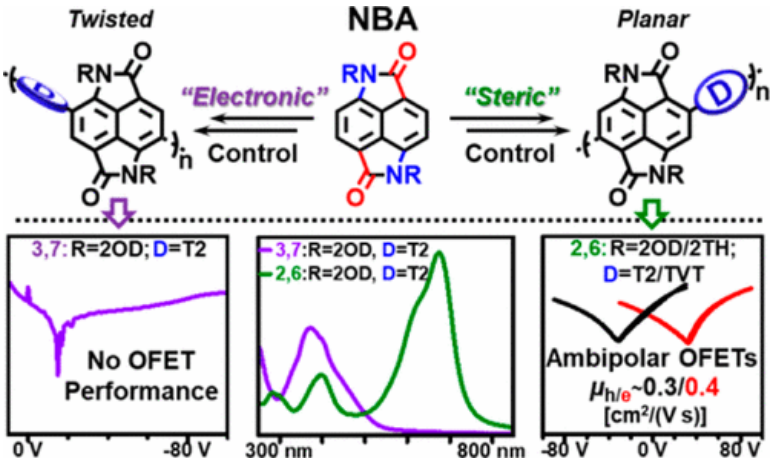
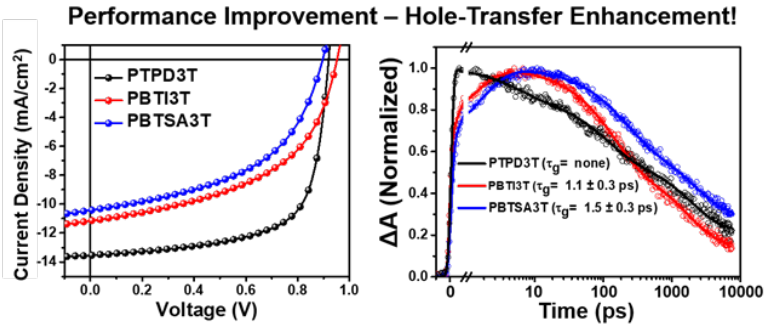


Caption: *Figure 6. Small Molecule Acceptor and Polymer Donor Crystallinity and Aggregation Effects on Microstructure Templating.*



Caption: *Figure 7. Naphthalene Bis(4,8-diamino-1,5-dicarboxyl)amide Building Block for Semiconducting Polymers.*



Caption: *Figure 8. Hole-Transfer Dependence on Blend Morphology and Energy Level Alignment in Polymer:ITIC Photovoltaic Materials Probled by Transient Absorption Spectroscopy.*

Scientific Achievement

How OPV donor polymer molecular mass, aggregation tendencies of crystallinity (semicrystalline or amorphous), and templating phenomena affect the formation of optimum nanoscale bulk-heterojunction morphologies is poorly understood and holds the key to rationally increasing solar cell power conversion efficiencies and manufacturability, especially for post-fullerene cells (Figure 6). To address these issues, we developed a new readily scaled, synthetically flexible naphthalene bis (4, 8-diamino-1,5-dicarboxyl) amide (NBA) electron-accepting building block (Figure 7). NBA-based polymers were synthesized and demonstrated to have n-type behavior with high electron motilities approaching 0.5cm$^{2/}$Vs. Importantly, NBA polymers are strong light absorbers with medium-to-low band gaps and strong π face-on thin-film nanodomain orientation. In related work, OPVs were fabricated by pairing the small-molecule strongly light-absorbing post-fullerene acceptor ITIC with high fill-factor donor polymers developed by the Marks group. The resulting photovoltaic materials were examined by a wide range of structural/morphological and exciton dynamic characterization techniques. It is found by transient absorption spectroscopy (Figure 8) that power conversion efficiencies (>10%) closely track ultra-fast exciton separation rates and phase separation domain sizes.

Significance

With development of new post-fullerene acceptor materials affording record OPV power conversion efficiencies, studies focused on understanding fundamental principles of donor-acceptor "mixing" in bulk heterojunction blends becomes critical both for further power conversion efficiency increases and for achieving goals regarding long-term OPV device stability. The research presented in section IIA (Figures 6 and 8) establishes new guidelines for materials choices and processing strategies to form optimal high-performing blend morphologies. In addition, naphthalene bis(4,8-diamino-1,5-dicarboxyl)amide building blocks (NBA) enable new very valuable and rare n-type (acceptor) polymer materials for bulk heterojunction OPVs (section IIA, Figure 7). Due to increased and red-shifted light absorption versus incumbent naphthalenedimide acceptors, we envision NBA-based polymers being leading n-type materials for variety of semiconducting applications, but especially photovoltaics.

Citation
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