Interactions Between Non-Fullerene Acceptors Lead to Unstable Ternary Organic Photovoltaic Cells

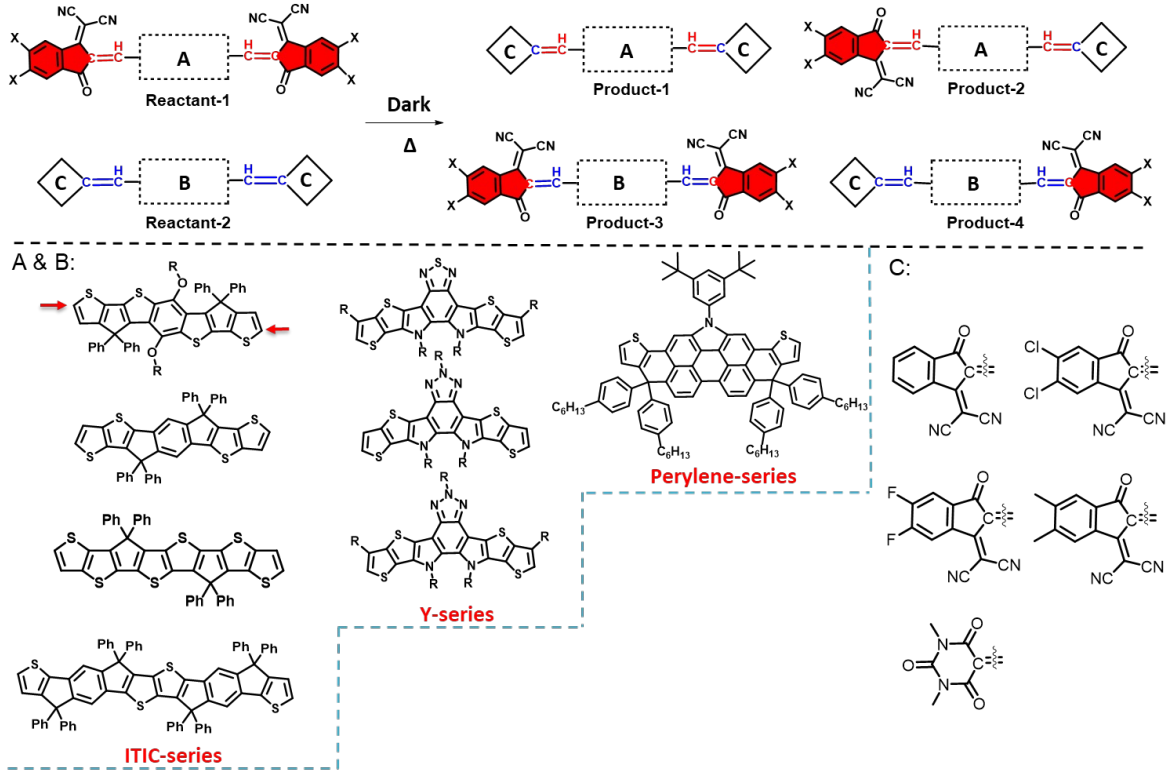

Figure: Generality of the end-capping exchange reaction between A-D-A non-fullerene acceptors. The top panel displays the end-capping exchange reaction between two A-D-A non-fullerene acceptors (NFAs). The vinyl groups linking the D and A moieties can dissociate at elevated temperature used during the mixing of the blend prior to forming the bulk heterojunction (BHJ) thin film. The exchange process results in reaction products with both asymmetric and symmetric molecular structures. Consequently, ternary-blend organic photovoltaics (OPVs) based on two NFAs and a donor can comprise up to seven chemical species.

Objective

- To gain a fundamental understanding of the mechanisms governing the stability of OPV devices based on A-D-A type non-fullerene acceptors (NFAs)
- To provide a guide to finding reliable organic photovoltaic materials

Impact

We demonstrate that almost all NFAs used in high efficiency OPV cells undergo H2O-catalyzed dissociative reactions during blending that create a plethora of reaction products. In ternary blend OPVs, if two NFAs are blended in a solution at elevated temperature, the acceptor end capping groups exchange between the molecules, creating at times up to 6 NFA molecules within the bulk heterojunction mixture. These reaction products have significant impacts on charge extraction efficiency, film morphology, photogeneration dynamics, and degradation of the performance under operation. These results provide insights into molecular designs and can explain the poor reliability and reproducibility of OPV devices other than the ternary blend devices discussed here.

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Relevant Papers

- Yongxi Li, et al., *PNAS*., 2023, under revision.

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