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Abstract

The efficiency of Organic Solar Cells (OSCs) has surpassed 18%, after a new generation of Non-Fullerene Acceptors (NFAs), the Y-series, was introduced to the field. These materials are characterised by high electron mobility, which is commonly attributed to its 3-dimensional packing motif in the single crystal. However, the bridge that links the NFA packing from single crystals to solar cells has not clearly been shown yet. In this work, we investigate the molecular organisation of a large body of NFAs, following the evolution of their packing motif in single-crystals, powder, and thin films made with pure NFAs and donor:NFA blends. We identified the most relevant packing motifs and polymorphs for the NFAs, discussing their role in the bulk heterojunction morphology, performance and charge transport, by combining experimental and theoretical approaches.

Conference Presentation