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Simultaneously Achieving Highly Efficient and Stable Polymer:Non-Fullerene Solar Cells Enabled By Molecular Structure Optimization and Surface Passivation

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Dedicated to Professor Baowen Zhang on the occasion of her 80th birthday.

Despite the tremendous efforts in developing non-fullerene acceptor (NFA) for polymer solar cells (PSCs), only few researches are done on studying the NFA molecular structure dependent stability of PSCs, and long-term stable PSCs are only reported for the cells with low efficiency. Herein, the authors compare the stability of inverted PM6:NFA solar cells using ITIC, IT-4F, Y6, and N3 as the NFA, and a decay rate order of IT-4F > Y6 ≈ N3 > ITIC is measured. Quantum chemical calculations reveal that fluorine substitution weakens the C═C bond and enhances the interaction between NFA and ZnO, whereas the β-alkyl chains on the thiophene unit next to the C═C linker blocks the attacking of hydroxyl radicals onto the C═C bonds. Knowing this, the authors choose a bulky alkyl side chain containing molecule (named L8-BO) as the acceptor, which shows slower photo bleaching and performance decay rates. A combination of ZnO surface passivation with phenylethanethiol (PET) yields a high efficiency of 17% and an estimated long T_{80} and Ts_{80} of 5140 and 6170 h, respectively. The results indicate functionalization of the β-position of the thiophene unit is an effective way to improve device stability of the NFA.

1. Introduction

With the advantages of being light-weight, flexibility, and solution processability, polymer solar cells (PSC) have received widespread attention and become a promising new generation of solar cells.[1] During the past few years, various high-performance polymer donors[2] and non-fullerene acceptors (NFAs) have been developed,[3] and power conversion efficiency (PCE) of PSCs have reached 18% rapidly.[4] In fact, the breakthrough of A-D-A type non-fullerene acceptors are the key to the leap in device PCE.[5] Through donor–acceptor structure modifications,[6] functional group substitution,[5c] and side-chain engineering,[7] various high-performance NFAs were developed and studied. DC-IDT2T was first reported by Zhan et al. as the A-D-A type NFA in PSC, where the indacenodithiophene (IDT) unit was introduced as the π-conjugated central donor moiety and 1,1-dicyanomethylene-3-indanone as the terminal acceptor unit (Scheme S1, Supporting Information).[8] Fusing IDT with two thiophene at both sides yielded a new acceptor molecule ITIC (**Figure 1**a).[9] By introducing two fluorine atoms on the benzene ring of 1,1-dicyanomethylene-3-indanone unit, Hou et al. reported a new NFA IT-4F (Figure 1a).[5c] The smaller optical band gap of IT-4F is beneficial for PSC since this increases the light harvesting ability of the blend,[10] making

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