Molecular Design of Non-fullerene Acceptor Materials for High Performance Solar Cells

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Recent progress on non-fullerene acceptor development has led to synchronous advances in polymer solar cells (PSCs) research, e.g. the power conversion efficiencies (PCEs) have been rapidly improved from 3% to state-of-the-art ~ 8%. To further boost the PCEs of device, non-fullerene materials utilize different region of lights and allow stacking into tandem device become one of attractive strategies. In this presentation, our recent molecular design and efforts addressing these issues are presented. A series of indacenodithiophene (IDT) unit-based non-fullerene acceptors are discussed regarding to their structure/device performance relationships. For instance, the 3-(dicyanomethylidene)indan-1-one moieties terminated at both sides of the indacenodithiophene-indacenodithiophene (IDT-IDT) unit endows molecules with narrow optical band-gap (E_g~1.5 eV), high electron mobilities, good solubility and amorphous nature in film, which provide a high performance (beyond 7%) over a simple processing. In addition, high performance active materials required optimal light-absorption and energy levels of molecules, which in turn can be efficiently tuned by engineering the conjugation length of monoric units or addition of strong electron-withdrawing unit. Through device, spectroscopy and theoretical analysis of photon-to-electron quantum efficiency for these analogous of non-fullerene materials, we demonstrate the correlation and limit between molecules structure/device performances, which may provide significant insight for new generation of material design.