Novel highly efficient non-fullerene acceptor based on naphtho[2,3-*b*]thiophene diimide for organic solar cells

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Organic solar cells (OSCs) have seen a tremendous investment and enthusiasm in the recent years due to its increasing power conversion efficiency (PCE) of up to 14% and lifetime exceeding a few years. With unique properties such as device flexibility and low cost, OSCs are emerging as an efficient complementary counterpart to inorganic solar cells. However, major limitations such as their poor stability and their limited efficiency still need to be surpassed. As most of these limitations come from the use of fullerene derivatives as one of the key active materials, non-fullerene acceptors (NFAs) have been receiving a lot of attention [1].

We herein report new NFAs based on indacenodithiophene (IDT) and naphtho[2,3-*b*]thiophene diimide (NTI), which show two strong absorption bands at 600−780 nm and 400−500 nm. With the NTI unit allowing easy functionalization on its imide part, we synthesized two differently substituted IDT-NTIs: 2-ethylhexyl (2EH) and 1-hexylheptyl (1HH). After careful device optimization in the combination with the complementary donor polymer PBDB-T, we achieved OSCs with PCEs higher than 9% and 5% for IDT-NTI-2EH and IDT-NTI-1HH, respectively [2]. These differences in the performances were explained by the influence of the substituents in the imide groups on the physicochemical properties and the crystalline nature in the blend films, and showcased the great influence of the branching point of the alkyl chains on the photovoltaic behaviors.

Encouraged by these promising results and the easy functionalization of the imide group, molecular design, synthesis, and evaluation of new NTI-based acceptors are now underway.

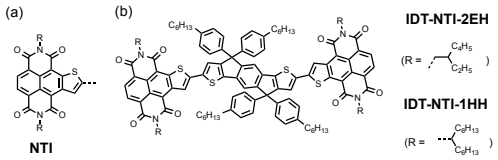

Figure 1: Chemical structure of a) the NTI building unit and b) IDT-NTIs and their terminations

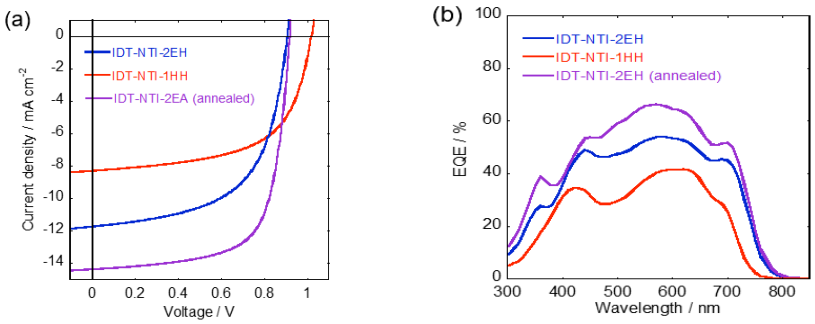

Figure 2: a) I-V curve of best OPV devices b) corresponding external quantum efficiency

[1] W. Chen, Q. Zheng, *J. Mater. Chem. C*, **2017**, *5*, 1275-1302 [2] J. Hamonnet, M. Nakano, K. Nakano, H. Sugino, K. Takimiya, K. Tajima, *Chem. Mater.*, **2017**, *29* (22), 9618–9622