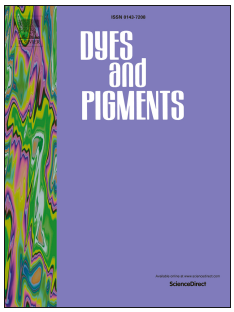
Accepted Manuscript



Alkyl side-chain and fluorination engineering in the indeno[1,2-*b*]fluorene-based small-molecule acceptors for efficient non-fullerene organic solar cells

Zhijing Lin, Kunxiang Huang, Zhaolong Wang, Xianjie Chen, Jing Sun, Zheng Xu, Tian He, Shouchun Yin, Miaomiao Li, Qian Zhang, Huayu Qiu

PII: S0143-7208(18)31573-0

DOI: 10.1016/j.dyepig.2018.08.039

Reference: DYPI 6953

To appear in: *Dyes and Pigments*

Received Date: 17 July 2018

Revised Date: 18 August 2018

Accepted Date: 20 August 2018

Please cite this article as: Lin Z, Huang K, Wang Z, Chen X, Sun J, Xu Z, He T, Yin S, Li M, Zhang Q, Qiu H, Alkyl side-chain and fluorination engineering in the indeno[1,2-*b*]fluorene-based small-molecule acceptors for efficient non-fullerene organic solar cells, *Dyes and Pigments* (2018), doi: 10.1016/j.dyepig.2018.08.039.

Alkyl side-chain and fluorination engineering in the indeno[1,2-*b*]fluorene-based small-molecule acceptors for efficient non-fullerene organic solar cells

Zhijing Lin,[†a] Kunxiang Huang,[†b] Zhaolong Wang,[a] Xianjie Chen,[a] Jing Sun,[a] Zheng Xu,[c] Tian He,[a] Shouchun Yin,[a] Miaomiao Li,[b*] Qian Zhang[a*] and Huayu Qiu[a*]

[a]College of Material, Chemistry and Chemical Engineering, Hangzhou Normal University, Hangzhou, 310036, P. R. China. E-mail: qzhang@hznu.edu.cn; hyqiu@hznu.edu.cn.

[b]School of Materials Science and Engineering and Tianjin Key Laboratory of Molecular Optoelectronic Science, Tianjin University, Tianjin 300072, P. R. China. E-mail: miaomiao.li@tju.edu.cn.

[c]Key Laboratory of Organosilicon Chemistry and Material Technology of Ministry of Education, Hangzhou Normal University, Hangzhou 310012, P. R. China.

[†]These authors contributed equally to this paper.

ABSTRACT

A series of non-fullerene acceptors based on the indeno[1,2-*b*]fluorene central moiety, with thiophene or 3-octylthiophene as π-bridge and either non-fluorinated or fluorinated 2-(3-oxo-2,3-dihydro-1*H*-inden-1-ylidene) malononitrile as end-capping groups (namely ICBF-O, ICBF, FICBF-O and FICBF), have been designed and synthesized. The effect of alkylation of the π-bridge and fluorination of the end-capping groups on the absorption spectra, energy levels, active layer morphology and photovoltaic performance were systematically investigated. Alkylation upshifts the molecular LUMO levels and thereby a high open circuit voltage (V_{oc}) of 1.06 V was obtained. However, the larger band gap induced by alkylation led to lower short circuit current (J_{sc}). Fluorinated acceptors display lower V_{oc} but higher J_{sc} and FF compared with non-fluorinated acceptors, coinciding with their lower LUMO levels, narrower band gaps and favourable morphology. As a result, the non-fullerene solar cells (NFSCs) based on FICBF showed the highest PCE of 7.41% among these four acceptors. The ICBF based device delivered a comparatively high V_{oc} of 0.99 V and a PCE of 6.07%. The results demonstrated that indeno[1,2-*b*]fluorene is a promising building block for efficient NFSCs.

Key words: non-fullerene acceptors, indeno[1,2-*b*]fluorene, alkylation, fluorination

1. Introduction