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

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### ABSTRACT

A series of non-fullerene acceptors based on the indeno[1,2-*b*]fluorene central moiety, with thiophene or 3-octylthiophene as  $\pi$ -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  $\pi$ -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

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