Development of New ITIC Isomers for Non-Fullerene Acceptors in Organic Solar Cells

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ITIC[1] is a representative non-fullerene acceptor (NFA) that has gained significant attention in OSC research due to its outstanding optoelectronic properties and flexible molecular design[2]. The molecular engineering strategies for the **ITIC** series include replacing terminal electron-accepting units, modifying electron-donating fused cores and regulating bulky side chains. Furthermore, the aggregation behaviors of molecules play a crucial role in determining the orbital energy levels of the aggregates, which in turn impacts the optoelectronic properties and OSC characteristics. Here, two types of **ITIC**-based NFA[3] (named, **im-ITI** and **io-ITIC**) with C_{2v} symmetry (Figure 1) were designed and synthesized to investigate the effect of molecular structure on the optoelectronic properties and OSC characteristics.

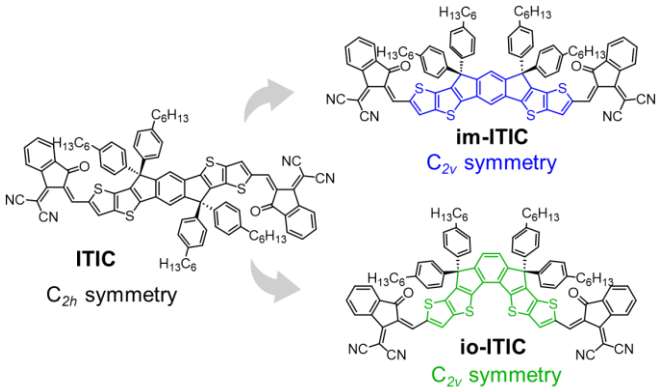

Figure 1. Molecular structures of **im-ITIC**, **io-ITIC**, and **ITIC**.

The UV-vis absorption spectra in film state of **im-ITIC**, **io-ITIC,** and **ITIC** showed maximum absorbance peaks at 637, 667 and 698 nm, respectively (Figure 2a). The OSC devices using **im-ITIC** as an acceptor and PBDB-T (CAS No. 1415929-80-4) as a donor showed a higher open-circuit voltage than that of **io-ITIC** and **ITIC** (Figure 2b) due to their different stacking modes and aggregation behaviors.

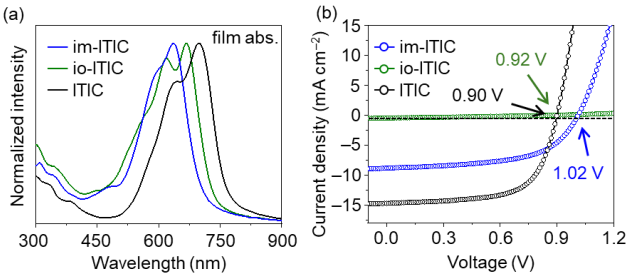

Figure 2. (a) UV-vis absorption spectra and (b) *J–V* curves of **im-ITIC**-, **io-ITIC**-, and **ITIC**-based OSCs.

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